



# **Abstract Book**

14<sup>th</sup> Biennial Electrochemistry Seminar of IRAN Kharazmi University



# In the Name of God

Green Chemistry Kharazmi University

Kharazmi University

چهاردهمین سمینار دوسالانه الکتروشیمی (وبینار)

CHARTER IS IN A

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انجمن شیمی ایران

# Biennial Electrochemistry Seminar of IRAN

Kharazmi University 29 & 30 August 2021

Webinar

تغران شيابان شعيد مفتح دانشگاه شوارزمي دانشكده ن

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محورهای سمینار: الكتروشيمي تجزيه اي حسكرهاى الكتروشيميايي سنتبك و ترموديناميك واكتشهاي الكتروشيميايي الكتروشيمي توليد و تخيره انرژي الكتروليز منعتى الکتروشیمی و اترژی های تجدیدیذیر خوردگی و آبکاری الكتروسنتز والكتروكاتاليز الكتروشيمي سبز الكتروشيمي محاسباتي نانو الكتروشيمي الكتروشيمي-فيزيك الكتروشيمي صنعتي زيست الكتروشيمى ساير موضوعات مرتبط با الكتروشيمي

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# 14<sup>th</sup> Biennial Electrochemistry Seminar of IRAN

# Organizers:



Kharazmi University



**Iranian Chemical Society** 



Research Institute of Green Chemistry Kharazmi University



### Welcome Massage from Scientific Chairman

Scientific conferences and seminars, especially the international ones, have long been important drivers of national development. They provide opportunities to establish collaborations with academics, experts, and industries, and exchange or develop novel ideas. They also provide new techniques, new types of equipment, and data to publish which ultimately contributes to the scientific development of the country. In present global situation, rapid growth of science and technology has had tangible and intangible effects on all aspects of human life leading to an increase in the diversity and variety of human needs and desires compared to the past. Chemistry is one of the most usable experimental science which we face it directly in everyday life. Thanks to chemistry, innovative products are improving the world around us and making our lives healthier, safer, more sustainable and more productive.

Electrochemistry has numerous uses in modern science and technology, including the production of vital industrial and pharmaceutical chemicals, covering various surfaces, and the plating and refining of metals. Also, the use of electrochemical methods in generation of clean energy is widely developed and is of great environmental importance. In this regard, On August 29 and 30, 2021, the Iranian Chemical Society will have its fourteenth biennial seminar on electrochemistry, which will be hosted by Kharazmi University, the Iran's first modern higher education institution. The safety of the participants is a top priority. Due to the coronavirus spread and in light of the health safety recommendations for Iran, this seminar goes virtual.

Decomposition electrochemistry; Electrochemical sensors; Bioelectrochemistry; Kinetics and thermodynamics of electrochemical reactions; Electrochemical physics; Electrochemical energy production and storage; Electrochemistry and renewable energy; Industrial electrolysis; Corrosion and plating; Electrosynthesis; Electrocatalysis; Green Electrochemical; Computational electrochemistry and nano-electrochemistry are among the 14 important specialized areas in the field of electrochemistry that will be covered during the seminar. This year's conference will attempt to bring in key speakers from around the world who are experts in the subject of electrochemistry. Workshops and industrial meetings will be held in addition to scientific lectures. Accordingly, professors, craftsmen, researchers, students and esteemed enthusiasts in the field of electrochemistry are invited to present their latest achievements and participate in this conference.

Electrochemical professors, craftsmen, researchers, students, and enthusiasts are cordially invited to exhibit their latest achievements and attend this conference. It is hoped that this conference will provide a suitable platform for presenting new perspectives, theories, and findings of electrochemical scientists in order to identify and solve Iran's serious problems and challenges in related industries. Let us take a decisive step toward the development, growth, and prosperity of our beloved Iran.

Mohammad Hossein Mashhadizadeh Professor of Analytical Chemistry Kharazmi University



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# **Keynote Speakers**





Title: Supercapacitor Electrode Materials Based on Metal-Organic Frameworks





# **Dr. Masoud Baghernejad**

Forschungszentrum Jülich GmbH, Helmholtz Institute Münster (HI MS, IEK-12), Münster, North Rhine-Westphalia, Germany Title: Electrochemical Gating of Single Molecules

# Dr. Hadi Khani

Texas Materials Institute, Cockrell School of Engineering, The University of Texas at Austin Title: Screening the Electrocatalytic Activities of Graphite-Coated Nickel, Cobalt, and Iron Nanoparticles and Their Alloys



# Dr. Soosan Rowshanzamir

Iran University of Science and technology, Iran Title: Hydrocarbon Based Polymeric Cation Exchange Membranes for the Chlor-Alkali Membrane Process



# Dr. Behnam Rasek

Energy and Environment Campus of Petroleum Industry Research Institute, Iran Title: Monitoring and Control of Microbial Corrosion in the Oil Industry



# Dr. Jaber Neshati

Energy and Environment Campus of Petroleum Industry Research Institute, Iran Title: Corrosion management in the National Iranian Oil Company

# **Oral Presentation**



# Convergent Paired Electrosynthesis of Symmetric Spiro-Pyrimidine Derivatives via the Generation of Appropriate Michel Acceptor from Para-Nitrophenol

### Mahmood Masoudi Khoram<sup>a</sup>, Nilofar Mohammadi<sup>a</sup>, Davood Nematollahi<sup>a, \*</sup>, Sadegh Khazalpour, Hossian Masoumi.

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A convergent paired electrochemical method was developed for the synthesis of new types of spiro and dispiro compounds in a good yield. Generation of the highly reactive intermediate from the electro-conversion of 4-nitrophenol (4-NPh) in the presence of barbituric acids (1a-1c) has led to the formation of target products (3a-3c). The results show the two different mechanisms for the conversion of 4-NPh in the electrode process. When the 4-NPh reduced via the four-electron process, the cathodically generated phenylhydroxylamine is oxidized at the anode to related nitrosophenol, while the six electron reduction of 4-NPh is produced 4-aminoaniline which converted to quinone imine after anodic oxidation. The reaction of the deprotonated form of barbituric acids with the nitrosophenol and quinone imine form the carbon-nitrogen and carbon-carbon bond in the final products, respectively. The highly symmetric spiro compounds (3a-3c) have been synthesized successfully in a safe water/ethanol mixture at the carbon electrode in an undivided cell using the constant current electrolysis method.



# C–C bond formation based on transition metal-catalyzed electrochemical processes

# Sadegh Khazalpour\*, Sara Torabi, Mahdi Jamshidi, Parvaneh Amooshahi, Maryam Mehrdadian

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The in-situ formation of various organometallic reagents by electrochemical methods for addition (carbon-carbon bond) reactions is discussed. In this study, the organometallic complexes are formed by the insertion of a metal in an alkyl or allyl halide structure. Furthermore, the catalytic cycles of the studied metals on the surface of electrodes and in solutions may consist of oxidative addition, the reductive elimination of ligands, metal transformation, the production of metal ions, or cyclization processes. Different types of C-C bond formation, such as Csp<sup>2</sup>-Csp<sup>2</sup>, Csp<sup>2</sup>-Csp<sup>3</sup>, and Csp<sup>3</sup>-Csp<sup>3</sup>, using transition metalcatalyzed and electrochemical approaches (organometallic electrochemistry) are discussed. Moreover, variety of metals, such as Zn, Ni, Sm, In, Mn, Ru, Pd, Fe, and Cr, are investigated as catalysts in the formation of C-C bonds between two organic compounds. High atom economy; excellent isolated yields; sustainability; scalability; one-pot, simple, and mild reaction conditions; and the non-toxicity of reagents are known as some unique features of the electrochemical protocols for the synthesis of organic compounds. In recent years, organometallic electrochemical reactions have aided the formation of one of the most important bonds in the synthesis of new molecules. Some of the most famous of these protocols are the metal-catalyzed or metal-mediated electrochemical Barbier, Nozaki-Hiyama-Kishi, Reformatsky, and Barbier-Grignard-type reactions. This study offers an overview of the application of strategies and methodologies based on electrochemical methods and metal catalysts for the allylation and alkylation of chemical compounds.

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# Determination of Atrazine Using a New Photoelectrochemical Aptasensor Based on AuNPs/g-C<sub>3</sub>N<sub>4</sub> Nanocomposite

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Atrazine (ATZ) is one of the highly toxic triazine herbicides, which is widely used in agriculture [1]. The widespread use of atrazine has been resulted in the release of this pesticide into the soil, wastewater and other water source. The long-time exposure to atrazine even at very little amount can damage the endocrine, reproductive, central nervous and immune systems [2,3]. Also, atrazine has the teratogen and carcinogen effects on humans [4]. The European Union has set a limit of 0.1  $\mu$ g/L atrazine in drinking water [5]. The US Environmental Protection Agency (EPA) has limited the concentration of atrazine to be 3 ppb in drinking water [6]. Therefore, the identification and quantification of atrazine in environmental samples is of great significance for public security.

In this research work, a new sensitive photoelectrochemical (PEC) aptasensor was developed for atrazine determination based on the surface plasmon resonance effect (SPR) of gold nanoparticles (AuNPs) deposited on a graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) film. The graphitic carbon nitride was synthesized through the heat treatment of melamine and urea and it was characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive X-ray analysis (EDX) and X-ray diffraction (XRD). The prepared AuNPs/g-C<sub>3</sub>N<sub>4</sub> nanocomposite exhibited higher photoactivity than g-C<sub>3</sub>N<sub>4</sub> under visible light irradiation. As the recognition element, the ATZ aptamer was immobilized on the AuNPs/g-C<sub>3</sub>N<sub>4</sub> nanocomposite through thiol-gold (S-Au) bonds. In the presence of atrazine, the formation of aptamer-ATZ complex restricts the electron transfer on the electrode surface and therefore the PEC signal decreases. The proposed PEC aptasensor showed an excellent analytical performance in terms of sensitivity, selectivity, reproducibility and stability for quantitative determination of atrazine with a wide linear range and low detection limit. In addition, the prepared aptasensor was used for determination of atrazine in real water samples and the satisfactory results were obtained which confirms the practical application of the proposed sensor.

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Investigating the photoelectrocatalytic performance of polyaniline-WS<sub>2</sub> nanocomposite for oxygen evolution reaction under solar irradiation

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In recent years, the photoelectrochemical (PEC) water splitting has attracted the attention of many researchers because during this process, the clean and renewable energy of the sun is converted into chemical energy using suitable semiconductor materials. Nanostructured metal sulfides (especially intermediate metal sulfides) such as CdS, ZnS, CuS, WS<sub>2</sub>, MoS<sub>2</sub>, FeS<sub>2</sub>, Bi<sub>2</sub>S<sub>3</sub> and their composites are suitable for photoelectrochemical water splitting due to their high optical absorption coefficient and suitable band gap. In this project, the polyaniline-WS<sub>2</sub> (PANi-WS<sub>2</sub>) nanocomposite was synthesized by in-situ oxidative polymerization and characterized by Raman spectroscopy, X-ray diffraction (XRD), and Field emission scanning electron microscopy (FESEM). The synthesized nanocomposite was coated on Ti substrate using Dr. Blade method and was used as a photoelectrode (working electrode). The saturated calomel electrode (SCE) and Pt plate were used as reference and counter electrodes, respectively. The photoelectrochemical performance of Ti/pure PANi, Ti/pure WS<sub>2</sub>, and Ti/PANi-WS<sub>2</sub> were investigated by linear sweep voltammetry (LSV), chronoamperometry (CA), and electrochemical impedance spectroscopy (EIS) toward oxygen evolution reaction



(OER) in dark and simulated solar irradiation (100 mW/cm<sup>2</sup>) in NaOH 1 M as electrolyte. The Origa flex 01A Galvanostat - Potentiostat was used for performing the electrochemical tests. The Ti/PANi-WS<sub>2</sub> photoanode had the highest photocurrent density (11.48 mA/cm<sup>2</sup>) compared to

Ti/pure PANi (0.74 mA/cm<sup>2</sup>) and Ti/pure WS<sub>2</sub> (7.86 mA/cm<sup>2</sup>) at 1 V vs. SCE under light irradiation. In the PANi-WS<sub>2</sub> nanocomposite, the matching of energy levels between PANi and WS<sub>2</sub> causes proper separation and transfer of produced electrons and holes. Therefore, the recombination rate of charge carriers is reduced and the photoelectrochemical performance of the nanocomposite is improved. This is also clearly seen in the EIS results. The charge transfer resistance ( $R_{ct}$ ) of Ti/PANi-WS<sub>2</sub> is lower than that of Ti/pure PANi and Ti/pure WS<sub>2</sub>.

In conclusion, the synergistic effect of PANi as organic semiconductor and  $WS_2$  as inorganic semiconductor makes PANi- $WS_2$  nanocomposite as a suitable photoelectrode with high efficient performance for oxygen evolution reaction (OER).

Keywords: Polyaniline, WS<sub>2</sub>, Solar light, OER, Photoelectrocatalyst.

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# Development of a nanoscale voltammetric genosensor for rapid detection of COVID-19

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The world is currently witnessing the third large-scale pandemic in the last two decades after the severe acute respiratory syndrome (SARS) in 2003 and the Middle East respiratory syndrome (MERS) in 2012. The novel pandemic, known as COVID-19, is caused by the very contagious severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) virus. Due to the emergence and rapid global spread of COVID-19, the quick and accurate detection of virus or disease is increasingly vital to control the sources of infection and prevent the extensive spread of the disease.

A voltammetric genosensor has been developed for the early diagnosis of COVID-19 by determination of RNA-dependent RNA polymerase (RdRP) sequence as a specific target of novel coronavirus. The severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) uses an RdRP for the replication of its genome and the transcription of its genes. Here, the silver ions (Ag<sup>+</sup>) in the hexathia-18-crown-6 (HT18C6) were used for the first time as a redox probe. Then, the HT18C6(Ag) incorporated carbon paste electrode (CPE) was further modified with chitosan and PAMAM dendrimer-coated silicon quantum dots (SiQDs@PAMAM) for immobilization of probe sequences (aminated oligonucleotides). The current intensity of differential pulse voltammetry using the redox probe was found to decrease with increasing the concentration of target sequence. Based on such signal-off trend, the proposed genosensor exhibited a good linear response to SARS-CoV-2 RdRP in the concentration range 1.0 pM–8.0 nM with a regression equation I ( $\mu$ A) = – 6.555 log [RdRP sequence] (pM) + 32.676 (R<sup>2</sup> = 0.995) and a limit of detection (LOD) of 0.3 pM. The standard addition method with different spike concentrations of RdRP sequence in human sputum samples showed a good recovery for real sample analysis (> 95%). Therefore, the developed voltammetric genosensor can be used to determine SARSCoV-2 RdRP sequence in sputum samples.

Key words: Genosensor; SARS-CoV-2 RdRP sequence; PAMAM@SiQDs; Signal-off

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### Design and Construction of Lanthanum Selective Electrode Based on Chemometrics Model and Experimental Evaluation

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The increase use of ion sensors in different fields leads to many intensive studies to introduce sensing materials in the construction of ion selective electrodes, particularly lanthanide sensors. Since the selectivity of ion selective sensors, directly depends on the stability constants of ion-ionophore complexes, we predicted the stability constants of lanthanum ions with different ionophores by the QSPR model, previously. Although the stability constant of complex between the ion and the ionophore is required to be high enough to produce a noticeable selectivity, this constant must not be so large that ions are tightly bound, making the complexation process kinetically irreversible, so the sensor exhibits long response time [1]. Based on previous studies, the useful rang of ionophore complex formation constants in an ISE is usually about  $10^4 - 10^7$ .

In this work, we designed a new selectophore, (N'-[(1E)-(2-hydroxy phenyl) methylidyne] benzohydrazide (HMBH) for lanthanum ion based on the predictive GA-MLR model. At the first, the stability constant of the lanthanum-selectophore complex was calculated using the proposed MLR model and Drogon software. Then the stability constant of the complex was determined by conductometric method in acetonitrile solvent and KINFIT program. The obtained results, 4/046 and 4/45 by theoretically and experimentally method, respectively, were satisfactory. Potential responses of lanthanum selective electrode based on HMBH as selectophore was evaluated by varying the amount of ionophore, plasticizer, and ionic additive. The electrode prepared with 6% ionophore, 61% nitrobenzene, 3% NaTPB as an additive, and 30% PVC has shown a Nernstian slope of 19.12 mV per decade to activities of La<sup>3+</sup> ions with a short response time of 10 s.

The sensor has shown an appreciable selectivity for La  $^{3+}$  ions in the presence of other lanthanide ions.

Keywords: Lanthanum selective electrode, Complex stability constant, QSPR, Design of selectophore

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# **Poster Presentation**

# Part 1

- Analytical Electrochemistry
- Electrochemical Sensors
- Computational Electrochemistry
- Nanoelectrochemistry
- Bioelectrochemistry



# An Electrochemical Sensor for Famotidine in real samples by using a carbon paste electrode modified with reduced Graphene Oxide and Cu<sub>2</sub>O Nanocomposite

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Famotidine is used to treat duodenal ulcers and quell their recurrence, gastric ulcer, gastro esophageal reflux disease, and Zollinger-Ellison syndrome [1]. Beside of formal applications with the onset of the Covid-19 pandemic, various drugs were used to reduce disease severity and mortality. One of the most promising drugs is famotidine. Wu et al. [2] predicted structures of proteins encoded by the SARS-CoV-2 genome and identified famotidine as one of the drugs reduce viral replication using computational methods. In this approach, carbon paste electrode modified by using reduced graphene oxide (rGO) and cuprous oxide (Cu<sub>2</sub>O). Because of its remarkable electrochemical characteristics and electrocatalytic activities, reduced graphene oxide has sparked a lot of interest in creating electrochemical sensors and biosensors over the last decade [3]. Copper oxides, such as CuO and Cu<sub>2</sub>O, have gotten a lot of interest as prospective options for electrochemical sensors because of their inexpensive cost and strong catalytic activity [4]. The modifier was characterized using Scanning electron microscopy (SEM), Infra red spectroscopy (FTIR) and X-ray diffraction (XRD). The size of Cu<sub>2</sub>O nanoparticles is about 30 to 90 nm that proved with FE-SEM and XRD.

The modified electrode was applied to determine famotidine. The linear range was 0.1  $\mu$ M to 50  $\mu$ M and detection limit was 0.0388  $\mu$ M. The effect of several parameters such as pH, potential window, and scan rate were optimized. In optimum conditions, differential pulse voltammetry was used for quantitative determination of famotidine in blood, urine and pharmaceutical real samples. The recoveries for this samples were, 109.19% 110.98% and 99.69% respectively.

Keywords: Famotidine, Electrochemical determination, Cu<sub>2</sub>O, Reduced graphene oxide

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# Design of electrochemical sensor based on copper oxide/N-doped reduced graphene oxide nanocomposite and ionic liquid for the determination of 4aminophenol

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4-Aminophenol (4-AP) is a necessary chemical used in industry to synthesize dyes, standard solvents, antioxidants, photography chemicals and petroleum additives. Large amounts of 4-AP are also utilized daily to produce organic substances [1]. The maximum limit of 4-AP in pharmaceuticals is 50 ppm (0.005%, w/w) by the United States. Therefore, it is necessary to develop simple and reliable methods for determination of 4-AP, for environmental protection and human health [2]. Graphene-based nanocomposites have drawn much more interests for modification of electrode surfaces in electroanalysis with the unique properties including good biocompatibility, large surface area, high electrical conductivity and excellent catalytic property. In addition, hydrophobicity, high viscosity, ionic structure, ionic conductivity, very low volatility and biocompatibility are among the properties of ionic liquids (ILs) making them attractive for electrode modification [3]. In this work, an electrochemical sensor for detection of 4-AP was developed based on the CuO/N-doped reduced graphene oxide nanocomposite and IL modified carbon paste electrode (CuO/N-rGO/CPE). The experimental results showed the wide linearity range, with lower limit (0.05  $\mu$ M) of detection for determination of 4-AP.

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### Non-enzymatic Textile Glucose Sensor Based on Fe Doped CuO

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Glucose concentration is usually measured in blood nowadays, but it may also be done in other bodily fluids such urine, sweat, saliva, tears, and exhaled air (1). The majority of commercial glucose sensors are enzymatic and rely on the enzyme glucose oxidase to oxidize glucose. These sensors have a high level of selectivity and sensitivity. As modifier materials for glucose oxidation electrodes, nanoscale metals, metal oxides, metal oxide doped composites, and organic and inorganic composite materials have been used (2). Textiles have been used as a substrate for wearable biosensors because they are biocompatible, pleasant, adaptable, and stretchy (3).

A non-invasive electrochemical textile glucose sensor was created using a carbon paste electrode modified with Fe doped on CuO (Fe@CuO). Fe@CuO was characterized using scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), electrochemical impedance spectroscopy (EIS), diffuse reflectance spectroscopy (DRS), and X-ray diffraction (XRD). Using cyclic voltammetry, amperometry, and electrochemical impedance spectroscopy, the electrochemical characteristics of a carbon paste electrode modified with Fe@CuO nanocomposite were studied. In alkaline solutions, glucose could be oxidized on the modified carbon paste electrode as an enzyme-free sensor, which has a superior bio-sensing performance toward glucose oxidation with high sensitivity, a broad detection range  $(2.5 \times 10^{-3} - 19.2 \times 10^{-1} \text{ mmol L}^{-1})$ , ( $3.83 \times 10^{-1}$ - 6.57mmol L<sup>-1</sup>), low detection limit ( $8 \times 10^{-4} \text{ mmol L}^{-1}$ ), good long-term stability, and excellent selectivity in alkaline solutions.



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### Determination of Sulfanilamide by Voltammetric Method Using Modified Glassy Carbon Electrode

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Sulfonamides are used against bacterial infections. Vaginal infections, urinary tract infections, sore throats, and some staph infections in humans can be treated with sulfanilamide. Long-term use of sulfonamides has been reported to cause certain side effects, such as emission, bleeding turbulence, allergic hypersensitivity reactions in humans, and carcinogenesis leading to hypothyroidism [1]. Electrochemical methods have low toxicity, fast response and easy operation. By modifying electrochemical sensors by conductive intermediaries, their sensitivity and selectivity can be improved. Nanomaterials with new and extraordinary properties are a new approach in science and especially in electrochemical sensors [2]. The GR-CuS nanocomposite with rough interface can provide sufficient spaces for the immobilization of redox proteins with close interconnection. The higher conductive GR and the excellent electrocatalytic activity of CuS can provide a favorable micro environment for electrochemical communication, which is suitable for the electrochemical application with fast electron transfer [3]. In this study, we synthesized copper sulfide and graphene nanocomposites and measured sulfanilamide in a real sample using electrochemical method and glassy carbon electrode modified with this nanocomposite. The Voltammetric results showed wide linear dynamic range and good detection limit (9 nM) for sulfanilamide.

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### Voltammetric Behavior of Doxorubicin at a Modified Glassy Carbon Electrode and its Determination in Real Samples

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Doxorubicin (DOX) is one of the most potent anti-cancer chemotherapeutic drugs used to treat a wide range of cancers, including stomach, bladder, breast soft tissue, prostate, and several others. Doxorubicin causes several side effects and also has unique heart toxicity. Monitoring of DOX concentrations has become increasingly significant to ensure the remedial virtue of doxorubicin drug as well as to prevent side effects [1]. Electrochemical sensors have received a lot of attention due to their superior aspects such as good selectivity, high sensitivity and fast response. Modification of electrochemical sensors with nanomaterials can improve the ability of these devices to analysis of compounds in biological samples. Meanwhile, copper sulfide nanoparticles have attracted the attention of researchers due to their special properties such as biocompatibility and high electrical conductivity [2]. Our proposed sensor offers a simple and fast method for measuring DOX in a short analysis time. This sensor is based on a glassy carbon electrode modified with copper sulfide nanoparticles and it was successfully used to detect and determine doxorubicin hydrochloride using voltammetric techniques in real samples. The Voltammetric results showed wide linear dynamic range and good detection limit (0.5  $\mu$ M) for doxorubicin.

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# Preparation of GCE Modified With CuS Nanoparticles and its Application In Voltammetric Determination of 5-Fluorouracil

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5-Fluorouracil drug is an effective antitumor agent is used to treat many types of cancer. It also shows unpleasant conditions such as heart toxicity and organ toxicity with increased oxidative stress and apoptosis [1]. Determining the anticancer drugs is widely used in modern pharmacotherapy of cancer patients because anticancer drugs show very different clinical behavior. Electrochemical methods are highly regarded due to their accuracy, precision, high sensitivity, and selectivity. In this regard, various methods have been used to modify the electrode surfaces to solve major problems of electrochemical methods. In recent years, nanostructured materials have been used to design modified electrodes due to their specific physical and chemical properties. Copper sulfide nanoparticles among metal nanoparticles not only increase electrochemical activity but also cost-effective [2]. In this work, we use copper sulfide nanoparticles to modify the surface of glassy carbon electrodes due to their unique properties. The Voltammetric results showed wide linear dynamic range and good detection limit (0.8 nM) for 5-Fluorouracil.

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# Electrochemistry Seminar of IRAN 2021

# An Electrochemical Sensor Based on Modified Glassy Carbon Electrode for the Determination of the Anti-Cancer Drug Methotrexate

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Methotrexate is a yellow anticancer drug that belongs to the folic acid group and has a structure comparable to folic acid. It can inhibit tumor cell synthesis and inhibit the growth and reproduction of tumor cells by inhibiting the production of dihydrofolate reductase [1]. Recently, CuS nanoparticles due to their morphology, low cost, metal-like electrical conductivity, excellent catalytic properties and ability to increase electron transfer velocities at the electrode surface have been used to build sensors and biosensors. Thero improve the conductivity and electron transfer rate for electrochemical applications, there is an urgent need to fabricate dispersed nanocatalysts with highly conductive support. By combining GR and CuS to obtain a composite, GR-CuS nanocomposite has exhibited synergistic effects with attractive properties [2]. In this research, we used electrochemical methods to measure methotrexate using a glassy carbon electrode modified with copper sulfide and graphene nanocomposite (GR – CuS). The Voltammetric results showed wide linear dynamic range and good detection limit (8 nM) for methotrexate.

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# Determination of MIR-200a as a Biomarker of Ovarian Cancer Using a ZnS Quantum Dots-Based label Free Electrochemical Genosensor

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One way to diagnose cancer is to use microRNAs (miRNAs) that act as a biomarker. Ovarian cancer is the fifth most common cause of cancer deaths in women. Research shows that the expression profiles of the miRNA-200a play an important role in the discernment of ovarian cancer. In this study, a label-free electrochemical genosensor was devised based on ZnS quantum dots functionalized with L-cysteine (Cys-ZnS-QDs) to detect miR-200a, as a specific ovarian cancer biomarker. The Cys–ZnS-OD was characterized by various methods. Cys–ZnS-QDs are electrodeposited on the glassy carbon electrode surface and applied as an appropriate substrate for immobilization of the DNA probe. The effective parameters in the preparation of the genosensor are optimized to improve its analytical performance. The analytical performance of the genosensor has been investigated using electrochemical impedance spectroscopy and the EIS data were fitted to a Randles equivalent circuit. The linear range and the detection limit of miR-200a were found to be  $1.0 \times 10^{-14}$  to  $1.0 \times 10^{-6}$  M and 8.4 fM, under optimal conditions. Further, the genosensor is utilized to detect the target complementary miRNA string from a single-base mismatch miRNA string. Finally, this label-free electrochemical biosensor was used to detect miR-200a in human plasma without using any amplification method.

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# Development of a wireless feeding system for highly efficient electrophotocatalytic degradation of organic pollutants from aqueous solutions

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## **Graphical Abstract**

Electrochemical oxidation has been an intriguing approach for the elimination of toxic organic and residual compounds, in wastewater treatment, even at low concentrations [1]. Electrochemical oxidation can be considered as a green method because it consumes electrons instead of chemical reagents used in conventional wastewater treatment approaches. Recently, new sorts of electrochemical applications without direct electrical connections have been developed, which are generally known as wireless electrochemical systems [2, 3]. The setup of a wireless electrochemical system consists of a bipolar electrode (BPE) (as a conductive object) positioning in the electric field without any direct electrical connection. we have presented a novel wireless electro-photocatalytic (WEPC) process for the degradation of an industrial model dye RO29A wireless electrochemical configuration comprises two titanium mesh sheets as its feeder electrodes feeding an anodic bipolar electrode that is coated by Dy<sub>2</sub>O<sub>3</sub>/graphite/TiO<sub>2</sub> electro-photocatalytic. It was found that this electrode configuration can improve the photo-electro catalytic activity, significantly, via the reduction of the recombination rate of electron/hole  $(e^{-}/h^{+})$  in the electro-photocatalytic resulting in the fast formation of oxidizing species ('OH, O'). The experimental parameters such as potential gradient, initial pH, and reaction time were optimized to achieve the highest degradation performance based on chemical oxygen demand (COD) results. At the optimized conditions, a decolorization efficiency of 98% was achieved within 120 min, much higher than that of a conventional two-electrode configuration (75%). The results also showed that the percent



degradation for the developed and the conventional systems are 65% and 29%, respectively. The results also showed that RO29 decay follows quasi-first-order kinetics. The developed WEPC is a simple setup that has considerable advantages such as high degradation performance, high energy efficiency, and the possibility of operation without supporting electrolyte and oxidation additives.

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# Development of Carbon Paste Electrochemical Sensors Modified With Moleculary Imprinted Polymers and Gold Nanourchins for determination of Chlorpyrifos

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Pesticides are compounds that kill an unwanted organism or inhibit their population by interfering with their reproduction process. Chlorpyrifos (CPF) (O,O-diethyl-O-3,5,6trichloro-2- pyridylphosphorothioate) is a crystalline organophosphate insecticide. As a low toxicity pesticide, CPF is widely used in agriculture to eliminate pests harmful to crops [1]. Carbon paste electrodes have same advantages such as high electrochemical reactivity, commercial availability, good mechanical rigidity, disposable, low cost, low technology and easy of modification. Molecularly imprinted polymers (MIPs) are synthetic polymers with a predetermined selectivity for a given analyte, or group of structurally related compounds, making them ideal materials to be used in analytical chemistry [2]. Gold Nanourchins (GNUs) are uniquely shaped gold nanostructures with uneven surfaces covered in nanoantenna-shaped spikes that cause a larger surface compared to uniform spherical gold nanoparticles [3]. Modification of carbon paste electrodes with gold nanoparticles and molecularly-imprinted polymers increase sensitivity ands elective recognition, respectively. In this work, firstly MIPs was synthesized, then GNUs, MIP, graphite powder and mineral oil was mixed and electrode was prepared. The DPV data showed that the obtained cathodic peak currents were linearly dependent on the chlorpyrifos concentrations in the range of 0.1–400.0  $\mu$ M, with the detection limit of 0.07  $\mu$ M. Finally, the obtained CPF-imprinted electrochemical sensor was applied to the selective detection of CPF in vegetable samples.

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# Ag doped NiO based non-enzymatic sweat glucose detection

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Enzymes are used in glucose sensors on the market. These sensors are chemically and thermally sensitive. Metal oxide sensors, which have a longer lifespan than enzyme sensors [1, 2], can be used as an alternative to enzymatic sensors. Sweat glucose monitoring can help to simplify the job and offer data for more accurate diagnosis and therapy [3].

As constructed, a non-enzymatic glucose sensor employs a carbon paste modified with Ag doping in a NiO (Ag@NiO) nanocomposite electrode. The electrocatalytic activity of Ag@NiO was studied using cyclic voltammetry, and glucose in an alkaline solution was monitored using a differential pulse voltammetry method.

The proposed sensor offers a linearity ranging from 4  $\mu$ M to 1 mM with a detection limit of 0.3  $\mu$ M, and also displays excellent selectivity, stability, and reproducibility. And its application for the detection of glucose in real samples has also been demonstrated successfully.

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# Application of Metal Oxide Nanoparticles for Electrochemical Determination of Creatinine

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In this work, an enzymeless creatinine sensor was prepared according to exploiting carboneous and metal oxide nanoparticles with different isoelectric point (IEP) values. The carboneous nanostructure and metal oxide nanoparticles with different IEPs made a hierarchical structure as a microenvironment for the adsorption of creatinine. The dissimilarities between the IEP values of creatinine and the carboneous nanostructure is the driving force for adsorption of creatinine on the surface. Therefore, creatinine with positive charge can be adsorbed on negative carboneous nanostructure and consequently interacted with metal oxide, which resulted in formation of creatinine-metal oxide complex.

The obtained complex leads to changing charge transfer resistance ( $R_{ct}$ ) and double layer capacitance ( $C_{dl}$ ) at the modified electrode surface. The preparation of modified surface was studied using Fourier-transform infrared spectroscopy (FTIR) and ultraviolet–visible (UV-Vis) spectroscopy. Also, the morphology of the prepared surfaces was evaluated using scanning electron microscopy (SEM). Analytical evaluation of the fabricated modified electrode using electrochemical impedance spectroscopy (EIS) indicated a good linear concentration range for measurement of creatinine in micro-molar scale.

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# Electrochemical Evaluation of Metal Oxide Thin Film in Creatinine Detection

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Creatinine is a waste product formed from creatine and phosphocreatine in muscles and removed from the body by kidneys at a relatively constant rate. Therefore, detection of creatinine in body fluids is utilized to diagnosis of kidney damage and the progression of kidney disease. In this paper, a new sensor was designed for detection of creatinine through the corporation of carboneous/metal oxide nanostructure thin layer on the fluorine-doped tin oxide (FTO) glass.

The hierarchical carboneous/metal oxide nanostructure was coated on FTO using spin coating and cyclic voltammetry (CV) methods, respectively. The prepared thin film was suitable for interaction between creatinine and modified surface. Characterizations of the designed sensor were done using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), ultraviolet–visible (UV-Vis) spectroscopy and scanning electron microscopy (SEM). Electrochemical impedance spectroscopy (EIS) was used for detection of creatinine in samples. The prepared sensor indicated a good linear range in micro-molar scale. The fabricated electrode can be applied as a promising sensor for creatinine detection.

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# Applicability of Aptamer-MIP Hybrid Receptor as a Sensing Interface in Fabrication of Ractopamine Aptasensor

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Ractopamine (RAC) is a 2-adrenergic agonist with anabolic features that promote skeletal muscle growth, decrease fat deposition and increase protein accretion in tissues. RAC is abusively used as livestock feed additives in many countries [1, 2] and its accumulated residues in animal tissues induce some potential risks for human health. Furthermore, the RAC may result in disorders in the human central nervous and cardiovascular systems and even cancer [3,4]. Considering the World Health Organization (WHO) statement on the prevalence of common human diseases arising from lack of access to safe food and the importance of the healthy food chain, tracking this illegal feed additive in biofluids is crucial [5]. This study reports the capability of a double recognition strategy based on the aptamer and molecular imprinting polymer (MIP) as an interface sensing for a highly selective RAC detection. Accordingly, a complex amino DNA aptamer specific to RAC and RAC was immobilized on a glassy carbon electrode (GCE) surface modified with silver nanoparticles (AgNPs). Then, a polymer layer was synthesized on the surface by electropolymerization of dopamine. By washing the surface with a suitable washing solution, the RAC was separated from the aptamer arm and empty cavities were formed on the surface to embed the MIP layer. The sensing relies on the fact that both the MIP and Apt act synergistically to trap RAC molecules highly selectively. The sensing surface fabrication steps were studied by some electrochemical techniques such as electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV). The aptasensor detected RAC in a wide linear range of 1 fM to 1.90 µM. The detection limit (LOD) value was calculated to be 330 aM, superior to all of the other reported methods



in the RAC sensing. RAC analysis in human blood serum and urine samples was successfully done.

Keywords: Aptamer, Ractopamine, Electropolymerization, Molecular imprinting polymer, Nanohybrid

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# Azolla-modified electrode for trace determination of four phthalic acid esters in aqueous samples via response reduction of Fe<sup>2+</sup>/ Fe<sup>3+</sup> pairs

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At this work, it was tried to design a sensitive and efficient electrochemical sensor for determination of some phthalic acids esters (PAEs) including dibutyl phthalate (DBP), dimethyl phthalate (DMP), bis(2-ethylhexyl) phthalate (DEHP) and dicyclohexyl phthalate (DCHP) in aqueous solutions. Briefly, the surface of the copper electrode was modified with azolla powder and electroencephalography gel. The modified electrode was characterized by differential pulse voltammetry (DPV), electrochemical impedance spectroscopy (EIS), field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FT-IR), Brunauer-Emmett-Teller (BET) analysis and energy dispersive X-ray (EDX) methods. In the presence of PAEs as electrode blocker, the differential pulse voltammetry (DPV) response of redox pairs of Fe<sup>2+</sup> and Fe<sup>3+</sup> was decreased proportional to increase in PAEs concentration. The experimental parameters including the concentrations of Fe<sup>2+</sup> and supporting electrolyte, pH of solution and modifier to gel ratio were optimized with central composite design (CCD). At the optimum conditions, linear relationships were found between the DPV responses and PAEs concentrations and the limit of detection (LOD) and limit of quantification (LOQ) values were obtained in the ranges of 0.2-0.4 µg L<sup>-1</sup> and 0.5-1.0 µg L<sup>-1</sup>, respectively. Good recovery percentages ranging 97.3-100.3 with RSD < 3.2 % suggested the proposed method for efficient, accurate and quick determination of PAEs in real water samples.

**Keywords:** Azolla modified electrode, Centeral composite design, Differential pulse voltammetry, Electrochemical sensor, Phthalic acids esters.



# **Electrochemical Sensing of Indole in Plasma Based on Pd Nanoparticles Modified Metal-Organic Framework Cr-MIL-101/Ionic Liquid Sensor**

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Indole is a versatile pharmacophore, a privileged scaffold and an outstanding heterocyclic compound with wide ranges of pharmacological activities due to different mechanisms of action [1]. Indole is a powerful antioxidant and it appears to be especially effective against breast and cervical cancer because of its ability to increase the body's breakdown of estrogen [2]. Over the past decade, chemists are increasingly attracted towards the studies on the pharmacological and therapeutic activities of indole containing compounds. Furthermore, the molecular structures of well-known drugs such as sumatriptan, tadalafil, fluvastatin and rizatriptan are based on indole frameworks [3]. Thus, developing a simple and fast and reliable method for the measurement of indole is of great importance.

In this work, a simple, sensitive and robust electrochemical sensor has been developed for ultratrace determination of indole. The proposed sensor was designed by incorporating of Ultra-Small Nano-Sized Palladium Particles Stabilized on Metal-Organic Framework Cr-MIL-101 (Pd@Cr-MOF) and 1-hexyl-3-methylimidazolium chloride (1H3MCl) in the carbon paste electrode (CPE). The synthesized Pd nanoparticles modified Metal-Organic Framework Cr-MIL-101 (Pd@Cr-MOF) was characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The modified electrode (Pd@Cr-MOF/1H3MCl/CPE) showed excellent sensitivity towards indole compared to the



unmodified electrode. Under optimized conditions, the modified electrode exhibited a linear response over the indole concentration range of 1 to 1100 nM, with a detection limit of 0. 3 nM. Moreover, the-sensor was successfully applied for the determination of indole in human serum sample. In addition, high performance liquid chromatography (HPLC) method was applied for the validation of the proposed electrochemical method for the determination of indole in human serum sample.

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# An Electrochemical Sensor Based On A 3D Spongin Scaffold-MnO<sub>2</sub> Nanostructured Composite For Sensing Of Xanthine

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A novel carbonized 3D spongin scaffold as a novel support for nanostructured manganese oxide (IV) (MnO<sub>2</sub>-Spongin) was prepared and applicability of this was evaluated in the modification of a carbon paste electrode (CPE). The CPE modified with the nanostructure, which is denoted as the MnO<sub>2</sub>-Spongin/CPE, was used as a sensor in sensitive determination one of the purine derivatives (Xanthine (XA)). The MnO<sub>2</sub>-Spongin/CPE was characterized by several important methods and certain important factors were optimized. Under optimal conditions, analytical characterizations including linear range (from 10.0 nmol L<sup>-1</sup> to 1.0 µmol L<sup>-1</sup>) with a detection limit of 3.0 nmol L<sup>-1</sup> were studied. The validity of the MnO<sub>2</sub>-Spongin/CPE was studied for a measurement in human blood serum sample as the real sample with satisfactory results. These acceptable results may be attributed to the unique nanostructure in the paste as an efficient platform with the capability of the creation of the active areas on the platform and increasing the surface area to proper puissance of the XA oxidation.

**Keywords:** Sponging scaffold, Manganese oxide, Nanostructured composite, Electrochemical sensing, Xanthine, carbon paste electrode.

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# Design and Fabrication of an Electrochemical Sensor for Cortisol Determination

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In this research, cortisol content of hydrocortisone tablets, urine and human saliva was analyzed through a new electrochemical method. Cortisol as the most famous hormone of corticosteroids family is secreted by the human adrenal glands and enters the bloodstream [1], [2]. Cortisol is famous as a stress biomarker which affects human health system[3], [4]. This compound can be considered as an electroactive material due to its chemical structure. However, it has not shown a strong signal on bare electrode in low concentration levels [5]. This compound has a strong reduction peak but poor oxidation one. But due to the interference of oxygen reduction with cortisol, it can be directly electro-analyzed if dissolved oxygen is removed from the medium [6],[7]. Hence, in this work, cortisol was analyzed through an indirect method. It was found that there is a chemical redox reaction between hydrazine and cortisol. Thus, hydrazine was used as a chemical reducing agent and electrochemical probe for analysis of cortisol. In order to have an enhanced oxidation peak on the surface of the electrode, nanocomposite electrode (carbon paste) based on chemically synthesized copper tungstate nanomaterials were used. Differential Pulse Voltammetric method vs. Ag/AgCl/KCl 3M as a reference electrode and graphite as counter electrode in phosphate buffer saline (pH=7) has been utilized. After the reaction of hydrazine with hydrocortisone, the resulting product has an ability to be oxidized

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electrochemically. Thus, the peak of hydrazine is reduced and the oxidation peak of the product appears. In order to improve the results, tungstate copper nanoparticles which synthesized by co-precipitation method were used. This nanomaterial facilitated the oxidation reaction at the electrode surface. The effective parameters such as potential sweep, electrolyte pH (acidic, neutral and alkaline aqueous conditions), modifier and concentration on peak voltammetry current has been investigated and optimized. The modified electrode has a fast and sensitive response in the wide linear range of 5-250 nM and with LOQ of 5 nM, as well as, LOD of 1.34 nM. The main advantages for proposed electrode was good repeatability, reproducibility, with RSD less than 2.15%. Finally, hydrocortisone content of some pharmaceutical formulation is analyzed successfully. In addition, human cortisol in urine and saliva samples (2 hours after waking up), was well analyzed through the suggested method.

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# Fabrication of a new electrochemical imprinted sensor for determination of ketamine based on modified polytyramine/sol-gel/f-MWCNTs@AuNPs nanocomposite/ pencil graphite electrode

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Ketamine, which is a phencyclidine analogue, is mainly used as an anesthetic drug that stimulate N-methyl-D- aspartate (NMDA) receptors on neuronal cells. It induces loss of consciousness, amnesia, immobility, pain relief and sedation while the cardiopulmonary functions and the protective airway reflexes remain unchanged [1]. Furthermore, ketamine is a popularly abused drug among teenagers due to its stimulant, dissociative and hallucinogenic effects [2]. The overdose of ketamine has been found to cause a variety of side effects such as dysfunctions of the nervous, urinary and cardiovascular systems [3]. Therefore, the identification and quantification of ketamine in biological fluids and pharmaceutical samples is of significant importance for clinical purposes, drug seizing and also controlling the industrial processes.

This research proposes a new strategy for measurement of ketamine through one-step electropolymerization of the molecularly imprinted polymer (MIP) composed of polytyramine (pty), sol-gel, functionalized multiwall carbon nanotubes@gold nanoparticles (f-MWCNTs@AuNPs) nanocomposite and ketamine on a pencil graphite electrode (PGE) by cyclic voltammetric (CV) technique. F-MWCNTs@AuNPs nanocomposite was entrapped within the polymer network to enhance the electron transfer rate and sensitivity of the fabricated sensor. The f-MWCNTs@AuNPs nanocomposite was synthesized by the chemical reduction method and its structure characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) and energy dispersive X-ray analysis (EDX). The electrochemical behavior of the modified electrode was investigated using cyclic voltammetry, electrochemical impedance spectroscopy (EIS) and square wave voltammetry (SWV) techniques. Under the optimized experimental conditions, the calibration curve of the MIP electrode was plotted and two dynamic linear ranges from 1.0 to 50.0 nM and 50.0 to 1000.0 nM, with a limit of detection (LOD) of 0.7 nM were obtained for quantitative measurement of ketamine in solution. The obtained results show that the proposed sensor has an excellent stability, good reproducibility and repeatability, and high sensitivity and selectivity towards the ketamine molecules. Furthermore, the electrochemical imprinted sensor was successfully applied for determination of ketamine in biological samples with satisfactory results. **References:** 

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# Electrochemiluminescence sensor for determination of antibiotic Ceftazidime

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Ceftazidime (CFZ) is one of the important cephalosporin antibiotics that is used for treatment of infections in human and animal. Although it is helpful for healing of diseases, this antibiotic has side effects and its determination in food and biological fluids is necessary. Different analytical methods have been used for detection of CFZ, but Electrochemiluminescence (ECL) technique has not studied for this aim yet. ECL has become one of the important analytical methods for determination of various analytes because of its high sensitivity and selectivity. Classical ECL Luminophores like Tris(bipyridine)ruthenium(II), are toxic and expensive. Therefore, it is essential to find the new luminophores for preparation of green and cheap ECL sensors. Carbon quantum dots (CQDs) recently considered to use as luminophores in ECL systems. Recent studies showed that Nitrogen doped CQDs (N-CQDs), have higher ECL signals in comparison with undoped CQDs. In this work, N-CQDs were synthesized by solvothermal method and were characterized by different methods like FTIR, HRTEM, EDX, etcet. Results showed that mean size of N-CDs are 5 nm and functional groups such as carboxyl, hydroxyl and amino are exist on their surfaces. ECL study was performed by ECL device using glassy carbon electrode. During the study, ECL signal quenching was related linearly to CFZ concentration. So an ECL sensor was prepared for determination of CFZ in milk. Linear range of determination was between  $1.0 \times 10^{-7}$  and  $1.0 \times 10^{-3}$  M and detection limit was  $2.3 \times 10^{-8}$  M. Stability, repeatability and selectivity studies showed that prepared sensor is applicable for determination of CFZ in real samples.

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# Electrochemical Determination of Tramadol Using Carbon Paste Electrode Modified with Nanoparticles of CdS and Graphene

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Tramadol is a powerful painkiller with high doses of addictive. Many methods have been reported for the determination of tramadol in pharmaceutical and biological samples [1-4]. Electrochemical sensors have shown greater advantages because of their fast analysis, wide variety, and low cost [3]. According to previous research, carbon paste electrodes using nanoparticles of CdS and graphene modifiers have not been used simultaneously to measure tramadol. In this study, a new modified electrode was proposed to measure tramadol by carbon paste electrode modified with graphene and CdS nanoparticles. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) methods were used to analyze the prepared electrode. The catalytic property resulting from the synergistic effect of these two modifiers not only increased the oxidation current but also reduced the oxidation potential of tramadol. Scan rate and pH effects on the performance of modified electrode were also investigated. The electron transfer coefficient ( $\alpha$ ) for the electro catalytic oxidation of tramadol and penetration coefficient of tramadol under experimental conditions were also evaluated. The linear calibration curve of tramadol was obtained within the linear range of 0.01-270.00 µM, and the detection limit was calculated as  $6.3 \times 10^{-9}$  M. Finally, the modified electrode was successfully used to measure tramadol in some real samples such as blood serum and pharmaceutical samples.

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# A New Electrochemical Sensor Based on Carbon Paste Electrode Modified by Kaolinite Nanoparticles to Measure Mefenamic Acid

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Mefenamic acid is a non-steroidal drug with anti-inflammatory, analgesic and antipyretic activity. Several methods have been reported for measuring mefenamic acid in pharmaceutical and biological samples [1-4]. In recent years, electrochemical methods have been reported for measuring mefnamic acid due to their simplicity, speed, high sensitivity and no need for derivation. In this study, a carbon paste electrode modified with kaolinite nanoparticles was used to measure mefenamic acid. Various electrochemical methods such as cyclic voltammetry, differential pulse voltammetry, electrochemical impedance spectroscopy, chronoamprometry and chronocholometry were used to measure and study the mefenamic acid behavior. The electrochemical effect of mefenamic acid on the modified carbon paste electrode with kaolinite nanoparticles and the unmodified carbon paste electrode was investigated. Some parameters such as scan rate, amount of kaolinite nanoparticles, pH effect on the electrode behavior and pulse height were optimized. The linear range of mefenamic acid concentration was in the range of 0.1 to 550.0 µM and the detection limit was 0.013 µM. In order to determine the selectivity of the method, the effect of interferences of different species was investigated. Mefenamic acid was measured with the above electrode in real samples such as tablets and blood serum.

**Keywords**: Carbon paste Electrode, Kaolinite nanoparticles, Mefnamic Acid, electrochemical impedance spectroscopy, Voltammetry

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# Early detection of multiple sclerosis (MS) as a neurodegenerative disease using electrochemical nano-aptasensor

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Multiple sclerosis (MS) is a progressive inflammatory disease (neurodegenerative), and diagnosis of this disease can prevent recurrence of the disease and side effects. A biomarker is used as an indicator in the diagnosis of diseases. MicroRNAs are small, non-coding RNAs that are abnormally expressed in many diseases and have been identified as predictive biomarkers for the early detection of diseases. One of the best diagnostic biomarkers of MS is miR-155. In this report, a sensitive, low-cost, non-label electrochemical nano biosensor is used to identify miR-155. The biosensor comprises a nanocomposite of single-walled carbon nanotubes (SWCNT) and polypyrrole (PPY) on the graphite sheet (GS) substrate which is assembled with aminated aptamer as miR-155 capture probe. The characterizations are done with Fourier transform infrared (FTIR) and field emission electron microscopy (FESEM). All electrochemical measurements are performed in the presence of  $Fe(CN)_6^{3-/4-}$  as a signal generating element in the solution. The biosensor has a dynamic range of 10 aM to 1 µM with a detection limit of 10 aM. According to the ease of preparation, almost low cost, and good repeatability and reproducibility the proposed biosensor can be a good candidate for early detection of MS., fabricated biosensor showed acceptable performance in human serum samples and also good selectivity indiscriminate between the complementary target and noncomplementary one, so this nano-genosensor can clinically be used for prostate cancer diagnosis through the detection of miR-155 in human serum samples

**KEYWORDS:** Multiple sclerosis (MS); miR-155; Electrochemical nano-geno sensor; Single wall carbon nanotube; Polypyrrole; Differential pulse voltammetry

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# Design an electrochemical immunosensor for the detection of prostate specific antigen by a voltammetric method based on the multiwalled carbon nanotube/L-histidine functionalized reduced graphene oxide nanoplatform

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In this study, a simple and lable-free voltammetric immunosensor was successfully developed for the ultrasensitive detection of prostate specific antigen (PSA). To do this, multiwalled carbon nanotube (MWCNT)/L-histidine functionalized reduced graphene oxide (His-rGO) was demonstrated as a bifunctional nanoplatform for covalently attaching thionine redox indicator and anti-PSA antibody (Ab). The MWCNT enhanced electrical conductivity and facilitated the electron transfer between thionine and the glassy carbon electrode. While, the presence of anti-PSA antibody blocked the electron transfer of thionine and decreased redox signals. The principle response of proposed immunosensor was based on the selective interaction of PSA with thionine-NH2-GO-COOH-Ab. This selective interaction led to further decrease of response current of attached electrochemical probe. The liner calibration curve for tumor marker determination was 10 fg mL<sup>-1</sup>–20 ng mL<sup>-1</sup> (R<sup>2</sup>=0.996). Under optimized conditions, the immunosensor was able to selectively detect PSA with a limit of detection (LOD) of 2.8 fg mL<sup>-</sup> <sup>1</sup> at  $3\sigma$ . The relative standard deviations (RSDs) for single-electrode repeatability and electrode-to-electrode reproducibility were less than 2.9% and 5.7% (n=5), respectively. Furthermore, the as-proposed immunosensor showed excellent performance in detection of PSA in the human serum and saliva samples, which implies that the current strategy has a promising feature for the clinical assessment of tumor marker status in patients with prostate cancer.

Keywords: Histidine-rGO; PSA; Saliva; Serum; Signal-off immunosensor

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# **`Electrochemical genosensor based on carbon nanotube/amine-ionic liquid** functionalized reduced graphene oxide nanoplatform for detection of human papillomavirus (HPV16)-related head and neck cancer

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In the present study, in an effort to the design and development of nanostructured carbon-based biosensors, an amine-ionic liquid functionalized reduced graphene oxide (NH<sub>2</sub>-IL-rGO) immunosensing nanoplatform for the electrochemical detection of human papillomavirus (HPV16) DNA in patients with HPV16-positive head and neck cancer (HNC) was reported. The model reaction considered in this work was based on grafting of imidazole to the surface of GO via its silvlanization with 3-chloropropyltrimethoxysilane followed by N-alkylation of imidazole and IL preparation. Then, the obtained NH<sub>2</sub>-IL-rGO was immobilized on a multiwalled carbon nanotube (MWCNT) modified electrode surface and, subsequently used for loading aminated DNA probes via covalent bonds by the glutaraldehyde (GA) reagent. In the presence of anthraquinone-2-sulfonic acid monohydrate sodium salt (AQMS) as a redoxactive DNA intercalator, the hybridization of ssDNA probes with the target HPV16 DNA strands (complementary strands) led to a significant increase in the genosensor response. The strong specific interaction between the immobilized probe chain and the complementary chain enabled the detection of the HPV16 gene with the differential pulse voltammetry (DPV) measurements. The described method provided an excellent accuracy and good selectivity, compared to the existing methods. This low-cost genosensor can detect ultralow concentrations of HPV16 DNA with a limit of detection of 1.3 nM (at  $3\sigma$ ) and a linear range of 8.5 nM-10.7 µM. To validate the accuracy and performance of method, the extracted clinical sample DNA was used on the pDNA-modified electrode unlike other works that used PCR products.

**Keywords**: HPV-HNSCC; Hybridization; Functionalized reduced graphene oxide; Signal-on genosensor

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# Designing a flexible and wearable glucose sensing platform based on Nickel-Cobalt sulfide synthesized via Microwave-assisted method

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Flexibility and human-body compatibility have been emerged through the use of commercial fabrics (CFs) in designing wearable non-enzymatic glucose sensing platforms. In this work, electrodes fabricated through direct synthesis of ternary nickel–cobalt sulfide nanostructures (Ni-Co-S NSs) on the CFs (Ni-Co-S@CFs) using a fast and facile one-step microwave-assisted method for this purpose. Fabrication was followed by the structural and electrochemical characterization of the electrodes. The glucose-sensing ability of the prepared wearable electrodes was investigated via cyclic voltammetry (CV) and amperometry techniques in alkaline media. Two linear-responses in wide detection ranges of 0.04–2.3 and 2.31–9.91 mM with the sensitivities of 628.1 and 242.8  $\mu$ A mM-1cm–2, respectively, together with a relatively low detection limit of 28.7  $\mu$ M (based on S/N = 3) were obtained. Sensors showed high selectivity, acceptable repeatability, and long-term stability. The glucose level in human serum samples was further determined by employing the fabricated Ni-Co-S@CFs. Encouraging performance together with the flexible and foldable design make the fabricated sensing platforms immensely promising for wearable sensing applications.



# electrochemiluminescence sensing of L-tryptophan based on graphitic carbon nitride nanosheets

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L-tryptophan (L-trp) plays an influential role in human growth and metabolism, which has a critical aromatic non-polar amino acid indole side chain (including an  $\alpha$ -carboxylic acid group and an  $\alpha$ -amino acid group)[1]. Detection and determination of L-trp are essential because the body is not able to make it[2]; hence the regular use of pharmaceutical formulations and supplements is vital for human bodies, and metabolic disorders of L-trp can cause insomnia, anxiety addiction, Alzheimer's disease, and obesity[3]. Herein, a novel ultrasensitive electrochemiluminescence (ECL) sensor for L-tryptophan (L-trp) detection based on the interaction between graphite carbon nitride nano-sheets (g-C<sub>3</sub>N<sub>4</sub>) and potassium persulfate (K<sub>2</sub>S<sub>2</sub>O<sub>8</sub>) on the surface of glassy carbon electrode (GCE) was introduced. ECL happens when the species get high-energy electron-transfer reactions on the electrode's surface and then form excited states, which later go to relaxation state through light emitting[4]. Here in this project, a new ECL sensor has been developed for rapid and straight forward L-trp detection based on



K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> as co-reactant with sulfate radical anion (SO<sub>4</sub><sup>•</sup>) generated during the reduction of S<sub>2</sub>O<sub>8</sub><sup>2-</sup> as intermediate participants and g-C<sub>3</sub>N<sub>4</sub> in the role of luminophore[5]. Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) was used as a semiconductor material, g-C<sub>3</sub>N<sub>4</sub> has become more and more fascinating in ECL sensors in recent years, which improves ECL efficiency because of its non-toxicity, simple synthesis process, low cost, and high photochemical stability[6]. Each role of these components in the measurement procedure was investigated by cyclic-voltammetry (CV). Under the optimal conditions, there is a linear relationship between ECL intensity and logarithm of L-trp concentration over a dynamic range of  $1.0 \times 10^{-14} - 1.0 \times 10^{-9}$  mol/L with a detection limit of  $6.8 \times 10^{-15}$  mol/L. This sensor displayed a low detection limit, long-term stability, high sensitivity and remarkable selectivity; also, it has informed a simple preparation system. As a result, this ECL method has excellent potential for L-tryptophan determination in pharmaceutical formulation.

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# Electrochemical Evaluation of a new Affinity-Based Platform for Biomacromolecular Sensing F. Ebrahimi <sup>a</sup>, S. A. Mozaffari <sup>a, \*</sup>, H. Salaramoli <sup>b</sup>

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Here supramolecular chemistry in combination with the priority of electrochemical techniques was employed for lactotransferrin biomacromolecule determination via analyzing the selective adsorption of this biomacromolecule onto the acidic functionalized gold plates (AFGP). The AFGP acts as a substrate to formation of coordinative complex which led to a considerable signal change in the differential pulse voltammetric (DPV) peak current of  $[Fe(CN)_6]^{3-/4-}$  redox probe due to interaction with lactotransferrin. Upon the recognition of the lactotransferrin via the formation of coordinative complex, the peak current decreased due to the electron transfer reaction restriction on the electrode surface. Under optimum condition, it was found that the proposed method could detect lactotransferrin at wide nanomolar concentration range with low detection limit. Furthermore, the capability of electrochemical impedance spectroscopy (EIS) as a simple and rapid alternative analytical technique for lactotransferrin detection was demonstrated.

**Keywords**: Lactotransferrin detection, Electrochemical sensor, Supramolecular chemistry, Bio-macromolecule.

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# Electrochemical detection of melatonin in body fluids based on graphitic carbon nitrides (g-C<sub>3</sub>N<sub>4</sub>)

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Melatonin (Mel, N-acetyl-5-methoxytryptamine) is a hormone which is secreted during the night from pineal gland, this indoleamine hormone is synthesized in the reaction between serotonin N-acetyltransferase and acetyl serotonin O-methyltransferase [1]. Melatonin has alternative roles in body, the most important role of melatonin is regulating the circadian sleepawake rhythms and the other roles such as: antioxidant effect as critical free radical scavenger [2], inflammatory hormone [3], neuroprotective agent in Alzheimer and Parkinson's diseases and it is also used in cancer therapy with controlling extra free radical activity [4], so melatonin is a vital agent for detection and determination. As mentioned before melatonin released from pineal gland and it exists in biological fluids such as blood, urine and saliva [5], so it plays important role in different biological process in the body. Therefore, during last decade detection of melatonin with convenient method is a challenge in different fields of sciences. In the past few years, different methods have been used for determination of melatonin such as ELIZA, spectrofluorimetric, micellar electrokinetic chromatography, radioimmunoassay (RIA), high-performance liquid chromatography (HPLC) with fluorometric or electrochemical detection, gas chromatography-mass spectroscopy (GC-MS), and chemiluminescence and electrochemical methods [6]. Between these alternative methods, electrochemical approaches have been attracted lots of attention during these years. Herein we functionalized a new sensor for melatonin determination based on multiwall carbon nanotubes, gold nanoparticles and



graphitic carbon nitrides (g-C<sub>3</sub>N<sub>4</sub>) as modifier on the surface of the glassy carbon electrode [6]. In the optimum conditions, this electrochemical sensor displayed a linear range of  $5.0 \times 10^{-7} - 1.0 \times 10^{-4}$  mol/L. Furthermore, the proposed sensor was successfully applied to detect melatonin in human plasma samples with excellent precision, remarkable selectivity and long-lasting stability.

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# Electroanalytical Determination of Carbendazim in Orange Juice Samples using Molecularly Imprinted Polymer based Gold Nanourchins Modified Carbon Paste Electrode

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Fungicides are a group of chemical compounds that are used to harm pests and consciously in the environment. Carbendazim (CBM) is a major constituent of benzimidazole and carbamate fungicides that widely used for several crops [1]. The development of modified electrodes in electrochemical methods has been considered by researchers. Carbon paste electrodes are a class of electrodes with a high physical stability, long lifetime, the versatility of chemical modification, miniaturization, and rapid renewal of the electrode surface. Molecularly imprinted polymers (MIPs) are synthetic polymers with a predetermined selectivity for a given analyte, or group of structurally related compounds, making them ideal materials to be used in analytical chemistry [2]. Gold Nanourchins (GNUs) are uniquely shaped gold nanostructures with uneven surfaces covered in nanoantenna-shaped spikes that cause a larger surface compared to uniform spherical gold nanoparticles [3]. Modification of carbon paste electrodes with molecularly-imprinted polymers and gold nanoparticles increase selective recognition and sensitivity, respectively. In this work, firstly MIPs was synthesized, then GNUs, MIP, graphite powder and mineral oil was mixed and electrode was prepared. The DPV data showed that the obtained cathodic peak currents were linearly dependent on the carbendazime concentrations in the range of  $0.1-600.0 \mu M$ , with the detection limit of  $0.05 \mu$ M.

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# Electrochemical Sensor Based on Imidazole Zeolites (ZIFs) and Gold Nanoparticles for the Determination of Nitrite

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Sodium nitrite (NaNO<sub>2</sub>) is a powerful oxidant. Which is harmful to the human body that causes diseases such as cancer. Children are more at risk than adults. This harmful substance can enter the human body in various ways, one of which is drinking water containing nitrite. Recently, this is one of the global challenges in protecting human health and the environment. Nitrite is also used in the pharmaceutical and agricultural industries. A new electrochemical sensor has been introduced in the present work. The proposed sensor is a nanocomposite of organic metal frames and gold metal nanoparticles that was easily designed and synthesized (core-shell ZIF-8@ZIF-67/Au NPs). This sensor was used for rapid measurement of high sensitivity nitrite. To measure nitrite, a glassy carbon electrode (GCE) modified with the proposed nanocomposite was used and was first time used to determine nitrite using differential pulse voltammetry technique (DPV). Organic metal frames were synthesized by a simple chemical method and after preparing the suspension of these synthesized samples, about 5  $\mu$ l were dropped on the electrode, and then the modified electrode was placed at room temperature for drying and in finally, gold nanoparticles were deposited electrochemically. Nanocomposite synthesized using transmission electron microscopy (TEM), Fourier transform (FT-IR), field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), ultraviolet spectroscopy, scattered X-ray spectroscopy Energy (EDX), and electrochemical element maps was detected. After the plot, the calibration diagram with the DPV technique, the detection limit, and the linear range was calculated for nitrite oxidation. The results also show that the proposed sensor has repeatability, good reproducibility, and excellent stability in nitrite determination. One of the successes of this sensor is in determining nitrite in water, sausage samples.

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# **Electrochemically Synthesis of Tungstate Bimetallic Nanoparticles; Application to Electrocatalytic Determination of Paracetamol**

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In this work binary cobalt-nickel tungstate nanoparticles (CoNiWO<sub>4</sub>-NPs) were electrochemically synthesized on the glassy carbon electrode. The electrodeposition of CoNiWO<sub>4</sub> was occurs in a two-step process. By applying a constant potential -1.4V (vs. SCE) to GCE in the solution contains Na<sub>2</sub>WO<sub>4</sub>, NiSO<sub>4</sub>, Citric acid, Ammonium oxalate, Co(NO<sub>3</sub>)<sub>2</sub> (pH=8.0) a ternary alloy of metals is first formed on the electrode surface. Binary nanostructures of cobalt-nickel tungstate was formed by applying potential sweeping in the range of -0.5 to 0.1 (vs. SCE) with a scan rate of 50 mVs<sup>-1</sup> for 15 cycles. The electrochemical synthesized nanoparticles have been characterize by using different techniques such as: X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), energy dispersive X-ray spectrometer (EDX) and elemental distribution maps. Electrochemical impedance spectroscopy (EIS) has been also used to determine electrocatalytic properties of CoNiWO<sub>4</sub> nanoparticles. The electrochemical behavior of paracetamol was studied on glassy carbon electrode modified with CoNiWO<sub>4</sub>-NPs. This sensor exhibits excellent electrocatalytic properties for oxidation of paracetamol. This proposed sensor was successfully used to determine of paracetamol in various samples including paracetamol tablets and syrup.

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# Electrochemical Water Oxidation by Mo and Mo/Au Nanoparticles Supported on Core-Shell Magnetic Nanoparticles

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In this research, we decided to immobilized Mo and Mo/Au nanoparticles on cellulosemelamine formaldehyde support and investigate its catalytic activity on the Water Oxidation process. For this goal, we prepared two catalysts through wet chemical and calcination synthesis way, the difference of catalysts limited to kind of nanoparticles only. The activity of the catalysts in electrochemical water oxidation were investigated with cyclic voltammetry between 1-2 volte with 0.05 volte scan rate in the 0.5 M H<sub>2</sub>SO<sub>4</sub> solution. The electrochemical investigation data showed that over-potential was the 670 and 680 mv for the Mo and Mo/Au catalysts respectively in the 10 mA.cm-2 current density. Unexpected, the electrocatalyst with Mo/Au nanoparticles showed poor activity than another Catalyst containing Mo nanoparticles only. This is maybe possible due to the negative interaction between Au nanoparticles and Cellulose-Melamine Formaldehyde substrate.

Keywords: Water oxidation, Metal nanoparticles, Renewable energy, Electrochemistry





# Study And Measurement Of Valine And Evaluation Of Its Parameters On The Surface Of Glassy Carbon Electrode

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The aim of this study was to develop a selective and sensitive electrochemical sensor for indirect measurement of value by a glassy carbon electrode. Hydroquinone acts as a probe. The electrochemical behavior of hydroquinone in the presence of an amino acid on the surface of a glassy carbon electrode indicates that hydroquinone is converted to quinone during a two electron/proton reaction. The amino acid with quinone in michael addition reaction. The differential pulse voltammetry demonstrated a linear range and limit of detection of value concentration from  $1.22 \times 10^{-11}$  to  $9.^{V} \times 10^{-11}$  and  $1.44 \times 10^{-10}$  to  $1.12 \times 10^{-9}$  and  $9.80 \times 10^{-12}$  M. Behavior and a high level stability during the experiments, making it particularly suitable for the analytical purposes.

This study aims at the electrochemical characterization of a novel sensor for determination of the valine on the surface of a glassy carbon electrode in the presence of hydroquinone as a probe was investigated using cyclic voltammetry and differential pulse voltammetry techniques. As one of the branched-chain amino acids (BCAA), valine is an essential nutrient for most mammalian species, it is one of the 9 essential amino acids that should be provided in the diet [1]. Notably, BCAAs such as valine are different from many other essential amino acids because they are primarily used in muscle and degraded but not in the liver [2]. Several reports have been found for the determination of valine using spectrophotometry and chromatography [3]. Due to the chemical structure of hydroquinone and its hydroxyl groups, the reduction potential of this compound is expected to depend on pH. The electrochemical response of hydroquinone was investigated using cyclic voltammetry in the wide range of pH from 4 to 11. First, hydroquinone is converted to quinone in the two electrons, two protons reaction, the second valine was react with the quinone in michale addition reaction. We are probably facing an EC reaction mechanism.

The optimal conditions for measuring value in the presence of hydroquinone are: scan rate=100 mV/s, pulse amplitude=25 mV, pH=7, potential range from 0.3 to -0.27 V. Linear dynamic range was obtained over the range  $1.22 \times 10^{-11}$  to  $9.^{\vee} \cdot \times 10^{-11}$  and  $1.44 \times 10^{-10}$  to  $1.12 \times 10^{-9}$  of value and the limit of detection was  $9.80 \times 10^{-12}$  M based on S/N=3 by differential pulse voltammetry. Finally the proposed method was found to have satisfactory repeatability, reproducibility and stability results with low relative standard deviation values. The developed method was successfully applied for the determination of value in biological samples.



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# Investigation And Evaluation Of Electrochemical Behavior Of Glycine On The Surface Of Glassy Carbon Electrode

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A novel and indirect voltammetric procedure for the selective determination of glycine is described. It is based on the oxidation of Hydroquinone (HQ) on an unmodified glassy-carbon electrode (GCE), generated by the selective reaction between glycine and Quinone. A single reduction peak of HQ at -0.1 V was observed, while glycine is not electroactive under this condition, showing that this reaction can be used to indirect detection of glycine. Under the optimized conditions, a linear response between  $1.20 \times 10^{-10}$  and  $1.08 \times 10^{-9}$  M and a detection limit of  $9.61 \times 10^{-11}$  M were achieved. The procedure is a promising alternative for rapid glycine determination in a wide range of samples.

Electrochemical techniques are also an alternative for glycine determination and exhibit some advantages in comparison to chromatographic techniques, such as low cost and simplicity for acquisition and maintenance. At the other hand, this technique shows adequate sensitivity for a variety of analytes in different matrices as well as easy miniaturization. Direct electrochemical glycine determination has not been reported until now [1]. However, this strategy has limitations because some oxidation products strongly absorb on the electrode surface. In the present work, a method for indirect glycine determination based on the electrochemical oxidation of HQ on a bare glassy-carbon electrode (GCE) is presented [2]. Electrochemical signal was formed by reacting HQ in the presence of glycine in BTR. This is the first report on the electrochemical oxidation of HQ for indirect determination of glycine.

Electrochemical measurements employing cyclic voltammetry (CV) and deferential pulse voltammetry (DPV) were performed using a potentiostat/galvanostat (Vertex, Ivium, Eindhoven, Netherlands) interfaced to a microcomputer and controlled by IviumSoft 2.5 software. A SCE and a platinum wire were used as the reference and auxiliary electrodes, respectively .In preliminary studies, electrochemical behavior of HQ and glycine was investigated by cyclic voltammetry, in the range of  $-0.\circ\circ$  to  $+\cdot.\circ\circ$  V, using a GCE and BTR as the supporting electrolyte. These results indicate that the selective determination of glycine is possible in the evaluated conditions. The reaction between glycine and quinone, was decreased the reduction current of HQ. Calibration curves were obtained using reference solutions containing increasing concentrations of glycine. A linear response was observed in the range of  $1.20 \times 10^{-10}$  and  $1.08 \times 10^{-9}$  M of glycine, described by the equation y=2224.1x+3.2411. The concentration of HQ in solution was  $3.31 \times 10^{-4}$  M. Limit of detection was achieved  $9.61 \times 10^{-11}$  M, based on S/N=3.





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# Determination of fexofenadine by voltammetry method at screen –printed electrode modified by graphene oxide nanosheets

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In this study, a rapid, simple and novel method has been developed to measurement fexofenadine. A screen printed electrode (SPE) the modified with graphen oxide nanosheets used to determine fexofenadine in sample solutions. The electrochemical oxidation of fexofenadine was investigated by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The oxidation of fexofenadine was irreversible. Different parameters (pH, concentration, scan rate, support electrolyte) were tested to optimize the conditions for the determination of fexofenadine. Under the optimum experiments condition (0.1 M KNO3 as support electrolyte, pH 7.0), the linear range was obtained for fexofenadine from  $3 \times 10-4$  to  $2 \times 10-7$  M with the detection limit (LOD) of  $2.1 \times 10-8$  M. The proposed method is unaffected, high sensitivity, and easy to use technic that successfully applied to determine fexofenadine in tablets and urine samples by a satisfactory recovery in the range of 95.2 to 1.4.5%.

Introduction: Fexofenadine is a histamine H1-receptor antagonist with the chemical name (+)-4-[1-hydroxy-4-[4-(hydroxydiphenylmethyl)-1-piperidinyl]-butyl]-(alpha),(alpha)-dimethyl benzeneacetic acid hydrochloride. It is a nonsedating antihistamine [1].

Result: In this method, by using graphen oxide nanosheets modified the surface of graphit screen printed electrode and measuring the analyte. Cyclic and Differential pulse voltammetry was used for determination of FEXO, voltammograms are shown in figure.1.

Conclusion:

A sensitive and selective electrochemical method for the determination of FEXO was established. After the optimization of some working condition, this method has been applied to the determination of FEXO in tablet and spike biological forms.



Figuer.1 cyclic (a) and differential pulse (b) voltammograms in different concentration of FEXO, at pH=7.0. The other experiments condition are as follows: scan rate = 100 mV/s, Tstep = 0.1s, Estep = 2mV.

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## Electrochemical Determination of Silymarin Using a Glassy Carbon Electrode Modified by Boron Nitride Nanosheet (BNNS-GCE)

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Herein, we present a novel electrode based on the research of the GCE electrode modified by Boron Nitride Nanosheet (BNNS/ GCE) for highlighted sensitive voltammetric measurement of Silymarin (SMR). The resulted BNNS/ GCE compound was characterized by means of powder X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive Xray analysis (EDX) and UV spectroscopy. Electrochemical performance of the modified electrode using cyclic voltammetry (CV), differential pulse differential voltammetry (DPV) and electrochemical impedance spectroscopy (EIS) to determine SMR in a phosphate buffer solution as a suitable electrolyte (pH 3.5 - 8.3) Was examined. The CV of the SMR in the potential range of -0.3 to 0.8 V showed reversible redox peaks that were pH-dependent. Processes meet reversible criteria.

We have optimized the conditions required for the practical demonstration of the new electrochemical sensor, where the redox peak current at pH 7.2 was linearly proportional to the SMR concentration in the range .012-0.160 mg/l<sup>-1</sup> with a detection limit of 0.09 mg/l<sup>-1</sup> (5% RSD) after 30 min of accumulation time by DPV. The reported sensor is suitable for analyzing small amounts of SMR in pharmacological drugs, plasma or urine.

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# Electrochemically induced cycloaddition reaction via anodic oxidation of acetaminophen in the presence of nucleophilic carbon compounds

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In pursuit of green methodologies in organic synthesis, electro-organic synthesis provides an effective and convenient one-step approach to organic transformations. In this report, an electrochemically induced cycloaddition reaction has been reported by anodic oxidation of acetaminophen in the presence of compounds in which the carbon atom has nucleophilic properties. Before electrochemical synthesis, electrochemical behavior of acetaminophene was studied in the absence and presence of acetylacetone as a nucleophile using cyclic voltammetry and controlled-potential and controlled-current coulometery. Based on these studies, the reaction condition including, pH, solvent (water/ethanol, v:v), number of transferred charge, etc., were optimized. Then, the reaction scope was explored via electrochemical oxidation of acetaminophen in the presence of various nucleophiles including acetylacetone, malononitrile and 1,3-cyclohexadione. These reactions were successfully performed using cathodic and anodic graphite electrodes by a controlled current system, in an undivided cell and products were obtained in good yield and purity. Further studies shown that these products could hold valuable pharmaceutical benefits.

**Keywords**: Electrosynthesis, acetaminophen, carbon atom nucleophiles, cycloaddition reaction.

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# Part 2

- Kinetics & Thermodynamics of Electrochemical Reactions
- Electrosynthesis
- Electrocatalysis
- Green Electrochemistry
- Physical Electrochemistry



# Fabrication of a pH-sensitive Coating Based on the Metal-Organic Framework of Caffeine@MIL-100 (Fe) as a Smart Anti-Corrosion Coating for Stainless Steel

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Corrosion of metals is a serious material degradation problem from economic standpoints, but it can to some extent be controlled by suitable strategies [1]. A new set of coatings named "smart coatings" serves as an impressive alternative for overcoming this problem. Corrosion inhibitors are loaded into nano/micro containers with high porosity. The inhibitors are then released under the influence of environmental stimuli and effectively decrease the corrosion rate [2, 3].

In this study, caffeine-loaded MIL-100 (Fe), caffeine@MIL-100 (Fe), was used as a smart corrosion-inhibiting coating to protect stainless steel (SS) in a 3.5 wt% NaCl solution. For this purpose, a thin film of the smart anti-corrosion caffeine@MIL-100 (Fe) coating was deposited on a SS surface using a decanoic acid self-assembled monolayer. The morphology and the structure of the synthesized MIL-100 (Fe) (as a metal-organic framework, MOF) were characterized by SEM, BET, XRD and FT-IR. A significant loading efficiency of 17.8% was obtained for caffeine loaded in the MIL-100 (Fe) framework. The acid-responsiveness of the coating was evaluated by the UV-Vis method. Based on the results, a decrease in the solution pH would cause the MIL-100 (Fe) MOF to decompose and subsequently release caffeine at the SS surface. The EIS results and the Tafel plots showed that the proposed smart coating has a good performance to protect SS from corrosion in saline media. The released inhibitor formed a protective layer on the SS surface and prevented the corrosive solution from penetrating into the substrate.

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# Electrochemical Synthesis of a new Metal-Organic Framework for Oxidation Processes

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Metal-organic frameworks (MOFs) are made by linking inorganic and organic units with stable bonds. The versatility with which the components' size, geometry, and functionality can be altered has led to more than 20,000 various MOFs being recorded and investigated within the past decade. The organic units are ditopic or polytopic organic carboxylates (and other similar negatively charged molecules), which, when linked to metal-containing units, yield architecturally strong crystalline MOF compositions with a typical porosity of more than 50% of the MOF crystal volume. The surface area values of such MOFs typically are high enough which exceeds traditional porous materials such as zeolites and carbons [1]. Electrically conductive MOFs are of significant interestfrom many attitudes. They are important as active substances for many purposes, including electro catalysis, chemiresistives ensing, and energy storage technologies. Their basic transport properties deserve further study; as certain conductive MOFs have been prognosticated to hosttopologically nontrivial electronic structures. Additionally, they may contain patterns of inorganic or organicmoieties that are unique in other materials, conceivablygiving rise to new physical phenomena. They also presentimpressive new avenues for creativity in ligand design, self-assembly, and crystal engineering. In this work, we synthesis Cobalt-based MOF and research its catalytic activities in electrochemical reactions. Electrochemical reactions are greener by using eco-friendly solvents, electrolytes, and economical precursors [2]. The result of using MOFs in electrochemical was meaningful. Firstly, the time of reactions reduces distinctly comparing to bare electrodes. secondly, capableness and yield have improved significantly. An increase in the surface area makes the reactants reach the surface cautiously and better [3].

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# Electrochemical Modification of Carbon Electrode and Investigating of Its Catalytic Performance

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Metal-Organic frameworks (MOF) are a class of crystalline or organic – inorganic hybrid compounds formed by coordination of metal cluster or ions with organic linkers, in which bivalent or trivalent aromatic carboxylic acids or N-containing aromatics are commonly used to form frameworks with zinc, copper, chromium, aluminum, zirconium, and other elements [1]. Organo- metallic compounds with uniformed and regular structures/adjustable porosity and different chemical properties have many applications including the following: gas storage and separation, heterogeneous catalysis, chemical sensing, biomedical sensing, biomedical application, and luminescence [2-3]. Various synthesis methods have been reported for MOFs/the most common of wich are: Solvothermal and Hydrothermal, Microwave, Sonochemichal synthesis, Mechanochemichal synthesis. In this study we use a mix of solvothermal technique and electrochemical protocol for fabrication of a new MOF. After preparation of the modified electrode we investigated its catalytic performance in chemical transformations.

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## A new Cobalt Modified Electrode for C-S Cross Coupling Reaction

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Metal-Organic Frameworks (MOFs) or coordinated networks constructed from metalcontaining ions and organic linkers are a special class of porous materials that have been attracted much attention in a wide variety of applications. There are many methods to synthesis such solvothermal, microwave synthesis, electrochemical **MOFs** as synthesis, Mechanochemical, and Sonochemical [1]. Each of these methods has some advantages and disadvantages. Due to its special features, the solvothermal method has attracted the attention of many research groups for the synthesis of MOFs, on the other hand, electrochemical methods for the synthesis of MOFs have also significant advantages, although they also have great challenges. Recently, the design of combined methods of electrochemical and solvothermal synthesis of MOFs has led to very interesting MOFs [2]. Generally, C-S crosscoupling reactions is catalyzed often by metal-based such as pd, Cu, Rh, and Ni [3]. Herein, we reported an efficient Cobalt-MOFs catalyzed C-S coupling reaction in high yields and selectivity. Utilization of the synthesized cobalt MOF led to a high reaction rate and a low-cost reaction procedure.

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## **Electrochemical alkylation of organic compounds**

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Organometallic reactions are approaches that can yield a broad spectrum of organic compounds, such as alcohols and amines, in aqueous and non-aqueous media [1,2]. The most applicable process of organometallic reagents is carbon-carbon bond formation (arylation and alkylation). In these protocols, the intended metals (zinc, magnesium, lithium, iridium, tin, chromium, nickel, palladium, copper, and ruthenium) are incorporated into the structures of organic compounds [3-5]. Electrochemistry and electrosynthesis are green and powerful tools for the investigation and synthesis of organic compounds. Also, the history of synthesis indicates that the application of applied current and potential (the electrochemical approach) in the synthesis of adducts is equally useful to organic chemistry and, in some cases, overcomes serious problems of the latter [6-9]. Organometallic reactions accompanied by electrochemical procedures have recently achieved considerable success in the formation of C–C bonds [10]. In this work, electrochemical alkylation of some diol compounds has been performed based on the paired process. The electrochemical reactions are different at the cathode and anode surface electrodes. At the anode surface, the diol compounds were oxidized via losing of protons and electrons. In contrast, the activation of alkyl halide is carried out at the cathode surface via the reduction of Ni (II) to Ni (0). In solution media, the coupling reaction between the oxidized form of diol compounds and activated alkyl halide was performed in non-aqueous media (DMF/LiClO<sub>4</sub>). The isolated products were identified and characterized via <sup>1</sup>HNMR, <sup>13</sup>CNMR, and FTIR spectra. In summary, we provided a new study of the metal-catalyzed electrochemical synthesis of organic compounds with C-C bond formation.

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## Photochemical Deposition of Silver Nanoparticles on TiO2 Nanotubes and Its Application for the Electrocatalytic Determination of Tinidazole

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Tinidazole is an antiparasitic drug used to treat some bacterial infections. Tinidazole has been studied because of its important role in numerous pathological processes. In this study, titanium nanotubes electrodes were decorated with silver nanoparticles (AgNPs/TiO2NTs) and used as an electrocatalyst for reduction of tinidazole. AgNPs/TiO2NTs are constructed by anodization of titanium sheet metal and photochemical deposition of AgNPs on TiO2NTs. Photochemical deposition is a green method for modifying substrates. The structural and elemental analysis characteristics of the AgNPs/TiO2NTs electrode have been studied by scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), and X-ray diffraction (XRD) methods. Based on cyclic voltammetric data, it has been confirmed that the AgNPs/TiO2NTs electrode has good electrocatalytic activity to reduce tinidazole. Using the amperometric method, the plot of the current of amperograms versus the tinidazole concentration has two linear segments (0.2-55.0  $\mu$ M and 55.0-111.2  $\mu$ M). A detection limit of 60.9 nM was obtained for measuring tinidazole at the AgNPs/TiO2NTs electrode surface. In addition, the designed sensor has been successfully used to quantitative measurement of tinidazole in pharmaceutical and human urine samples.

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# Clicked graphene oxide supported cobalt-polyoxometalate: An efficient water oxidation electrocatalyst

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Water oxidation catalytic processes have attracted intense attention due to their importance in energy storage as well as fuel production [1-5]. Oxygen evolution reaction during water oxidation is a complicated redox reaction which requires large oxidation potentials. Designing an effective, stable, and easily accessible catalytic system for water oxidation is very important for overcoming the global energy issue. Typical catalysts utilized for water oxidation involve the nanostructured catalysts as well as transition metal complexes [3-5]. Here, we develop a new hybrid nanomaterial based on the immobilization of cobalt containing polyoxometalate (CoPOM) on the surface of graphene oxide (GO) was designed for efficient electrocatalytic water oxidation reaction. First, graphene oxide (GO) was modified by cysteamine hydrochloride as linking agent via thiol-ene click reaction. Then, cobalt containing polyoxometalate, K<sub>6</sub>[CoW<sub>12</sub>O<sub>40</sub>], was supported on the surface of clicked graphene oxide through the electrostatic interaction with ammonium groups. The prepared material was characterized by Fourier transform infrared (FT-IR), X-ray diffraction (XRD), N2 adsorptiondesorption analysis, Transmission electron microscopy (TEM), Energy-dispersive X-ray (EDX), Scanning electron microscopy (SEM) and Cyclic voltammetry (CV). According to the results obtained by spectroscopy (FT-IR), it can be concluded that the surface of graphene oxide has been successfully modified through the covalent bonds. Based on nitrogen adsorption and desorption analysis (BET), significant reductions in the surface area of graphene oxide were observed due to the chemical modification and immobilization of polyoxometalate on the

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substerate surface. There are no characteristic peaks of (CoPOM) species in the X-ray diffraction patterns (XRD) of the heterogeneous electrocatalyst, indicating a good dispersion of polyoxymetals on the surface of catalytic support. TEM and SEM images showed that the layered-structure of the graphene oxide has been preserved after the chemical modification. Based on elemental analysis (EDX), the presence of polyoxometalate  $K_6[CoW_{12}O_{40}]$  in heterogeneous electrocatalysts was confirmed. Cyclic voltammetry (CV) showed the electroactive behavior of  $K_6[CoW_{12}O_{40}]$  by oxidation and reduction of cobalt (II) and (III). The achieved hybrid nanomaterial exhibited low overpotential of 155 mV vs. NHE at current density 10 mA.cm<sup>-2</sup> in the as electrocatalytic water oxidation at pH 7. In addition, a fast reaction kinetic with a Tafel slope of 85 mV.dec<sup>-1</sup> was seen in the presence of prepared hybrid nanomaterial. Linear sweep voltammetry (LSV) analysis revealed the long–term stability and activity of CoPOM–clicked GO for OER in neutral conditions.

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# Divergent Paired Electrosynthesis of Organic Compounds by the Co/Ni-BTC bi-Metallic MOF modified Electrodes

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The development of the efficient catalytic system for the electrosynthesis of organic compounds is not only an interesting issue in basic chemistry research, but it is also a significant case for the chemical industry. Remarkable attempts have been dedicated towards the employment of waste-free and selective synthesis of organic compounds. Metal-organic frameworks (MOFs) are the spotlight of a comprehensive research area, particularly as the modified electrode, with the eye-catching features of the large surface area and catalytic effects. This elegant idea can be accomplished by the paired electrosynthesis of organic compounds by MOF thin film modified (MOFTF) electrodes. In this work, we introduce the paired electrosynthesis of furoic acid and aniline via the Co/Ni-BTC bi-metallic MOF modified (bi-MMOF) electrode. To shed light on this issue, we used of cathodic electrodeposition technique for the synthesis and deposition of Co/Ni-BTC bi-MMOFTF on the carbon electrode. Then, the modified electrodes were employed for the electrocatalytic oxidation of furfural to the related acid and the electrocatalytic reduction of nitrobenzene to the related amine. From the green chemistry and eco-friendly standpoint, this strategy can be leads to the divergent paired electrosynthesis at the room temperature and green solvent with the enhanced energy, time economy, improved current efficiency and electrochemical yield. In the other words, two different substrates undergo synchronously oxidation and reduction to afford different products in one-pot reaction. Implementation of this eco-design procedure as a versatile protocol will be the first example of paired electrosynthesis of organic compounds with the Co/Ni-BTC bi-MMOFTF electrode.

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# Electrochemical Assay of diclofenac on an Ionic Liquid/MWCNTs Nickel Hexacyanoferrate Heterogeneous Electrocatalyst

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Diclofenac (DIC) is a well-known representative of non-steroidal anti-inflammatory drugs (NSAIDs) with strong anti-pyretic, analgesic and anti-inflammatory properties. Anti-inflammatory and analgesic properties of NSAIDs are widely exploited in the management of musculoskeletal diseases [1]. The development of sensitive and rapid method capable of determining drug amount in pharmaceutical and clinical monitoring is important. Up to now, many means and techniques have been employed for the determination of diclofenac sodium, such as chromatography [2], spectrophotometry [3], and electrochemical methods [4].

In this research, a sensitive voltammetric and impedimetric method based on 1-methyl-3butylimidazolium chloride (MBIMCl) ionic liquid - Nickel hexacyanoferrate nanoparticle (NiHCF) modified multiwalled carbon nanotubes (MWCNTs) nanocomposite (IL/NiHCF/MWCNTs) paste electrode was developed for the electrocatalytic determination of diclofentac (DIC) in real samples. The composite was prepared by a simple chemical method and was characterized by scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR), and atomic absorption spectroscopy. Also, the electrochemical behaviour of the modified electrode and the electrocatalytic oxidation of DIC were investigated in detail by cyclic voltammetry (CV), chronoamperometry and electrochemical impedance spectroscopy (EIS) techniques. The kinetic parameters such as electron transfer coefficient,  $\Box$ , and apparent rate constant for the redox reaction between DIC and the modified electrode were also determined using electrochemical approaches. It was found that the modified electrode exhibited excellent electrocatalytic activity toward the oxidation of DIC, and under the optimized conditions, the linear response range and detection limit were found to be 0.1-150.0 µM and 0.05 µM, respectively using the differential pulse voltammetry method (DPV). The

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proposed method was applied for the sensitive and selective determination of diclofenac in the urine samples and pharmaceutical formulations with satisfactory results.

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# Rapid and efficient electrochemical synthesis of a copper-based metal organic framework

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Metal–organic frameworks (MOFs) are a class of multifunctional porous materials which are composed of metal ions and organic linkers linked through coordination bonds. MOFs have gained considerable attention recently due to their intrinsic properties, such as high specific surface area, large pore volume, tunable pore size and high crystallinity [1]. These characteristics allow them to be suitable materials for applications such as catalysis, gas storage/separation, drug delivery, sensing, batteries, supercapacitors and water treatment, as well as photo- and electrocatalysis. Due to these widespread applications, the synthesis of MOFs has been extensively studied recently [2]. So far, several methods have been proposed for the synthesis of MOFs such as solvothermal, hydrothermal, microwave, mechanochemical, sonochemical and electrochemical. The electro-synthetic method of MOFs has some important advantages such as the easier handling, efficient reaction time and safety issue, which is potential to be applied in industrial scale.

This study focuses on thin film coatings of a promising Cu-based MOF material, known as  $Cu_3(BTC)_2$  [BTC = 1,3,5-benzenetriboxylate] (commonly known as MOF-199 or HKUST-1), which consists of dimeric copper paddle wheels linked by 1,3,5-benzenetriboxylates. First, 100 mL of fresh solution was prepared instantly prior to each reaction, comprising 50 mL deionized water, 50 mL ethanol, 1 g 1,3,5-benzenetricarboxylic acid as linker and 2 g of tributylmethylammonium methyl sulfate as conduction salt, which were stirred for half an hour till formed an homogenous solution. Then, the solution was heated to 50 °C, and after that the

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freshly polished copper electrodes ( $10 \text{ cm} \times 1 \text{ cm}$ ) were immersed into the solution, and applied a constant voltage (2.5 V) for more than 2 h to complete the reaction. Finally, the sky blue color precipitate of Cu<sub>3</sub>(BTC)<sub>2</sub> was collected from the electrolysis cell and dried overnight in a hot air oven at 120 °C. The structure of synthesized Cu<sub>3</sub>(BTC)<sub>2</sub> was characterized by X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FT-IR) was used to further investigate. The morphology of the prepared sample was examined by scanning electron microscopy (SEM), which confirms the cubic structure of the sample.

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## Electrochemical Study of 4-amino-N-(4-aminophenyl) benzenesulfonamide

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The synthesis of organic compounds by means of electrochemical methods have features that many of which cannot be achieved by other conventional methods. Most of electroorganic processes are performed under reagent-less and mild (atmospheric pressure and room temperature) conditions, one step using efficient and ecofriendly methods. In other words, electroorganic synthesis is in agreement with all the principles of green chemistry.

Aromatic amines constitute a major group of drugs which appear to be especially effective against bacterial infection (cefixime, ceftazidime, dapson), viruses (aciclovir, famciclovir), allergy (amprenavir, mesalazine, anileridine), cancer (bleomycin) and hypertension (amiloride, doxazosin). These compounds with antioxidative properties by prevention of oxidizing enzyme operation are led to repair the biological systems.

4-amino-N-(4-aminophenyl) benzenesulfonamide is important due to many applications such as an intermediate for dyestuff manufacturing, manufacture of azo dyes, pharmaceutical chemistry, leather dyes like acid black 210 and acid black 234. These introduces 4-amino-N-(4-aminophenyl) benzenesulfonamide as interesting class of compounds for further exploration. Following our experience in electrochemical synthesis of organic compounds based on oxidation and in situ generation of Michael acceptors, we were interested to develop some new class of 4-amino-N-(4-aminophenyl) benzenesulfonamide derivatives assisted by the electrochemical oxidation of 4-amino-N-(4-aminophenyl)benzenesulfonamide. In this work, we have investigated the electrochemical behavior of 4-amino-N-(4-aminophenyl) benzenesulfonamide via cyclic and linear sweep voltammetry. In the first step, the study of 4amino-N-(4-aminophenyl) benzenesulfonamide at different pH (1.0-12.0) showed anodic and I 4<sup>th</sup> Biennial Electrochemistry Seminar of IRAN August 2021



cathodic shift by increasing the basicity of the environment. Also, the reversibility of the system decreased via increasing pH and finally, at pHs 11.0 and 12.0, the system becomes generally irreversible. In the other word, in these conditions, the oxidized form of 4-amino-N-(4-aminophenyl) benzenesulfonamide participate in some side reactions such as hydrolysis or dimerization. For more data, some effective parameters such as the effect of scan rate, and concentration have been studied.

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# A review of the application of non-noble metals as electrocatalysts in the oxidation of methanol

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In the past decades, electro-oxidation of organic compounds such as methanol, ethanol, urea, glucose and glycerol has been considered by researchers. Nowadays, DMFCs due to their high theoretical energy conversion efficiency, low pollutant emissions, low operational temperature, high energy density, suitable storage, fuel transportation and easy operation are taken into consideration [1-2]. Typically, Pt-based noble metal catalysts have been extensively identified as the most capable electro-catalysts in DMFCs on account of their excellent methanol-oxidation activity, but the high cost and low utilization restrict their commercial applications [3-4]. As a result, exploring high activity non-noble metal catalysts in DMFCs is highly important and desirable.

Metal borides due to their interesting physical properties, as well as nickel boride compounds, as an important group of them, are always present in several phases, such as NiB, Ni<sub>2</sub>B, and Ni<sub>3</sub>B, which are currently Ni-B amorphous nanoparticles, have been used as electrocatalysts for the oxidation of alcohols.

Another case has been the use of  $CoS_2/MoS_2/rGO$ . Doping of  $MoS_2$  with metal ions and hybridization with reduced graphene oxide (rGO) have been performed to enhance its conductivity. The layered graphene increased the catalyst conductivity and decreased the charge transfer resistance. Thus, the electrochemical activity of the catalyst as an anode and cathode increased. The CV curve showed that with increasing methanol concentration from 0.05 to 0.3 M, the peak current density increased from 0.4 to 0.9 mAcm<sup>-2</sup>.

Another case was the use of NiCo<sub>2</sub>O<sub>4</sub> nanorods with high electronic conductivity and high ability to show a redox reaction, which was considered a very potential material for many vital applications. Further enhancement in the electrochemical performance could be achieved through morphology tuning or tailoring, as the electrocatalytic performance is largely reliant on the electrode material's morphology. The NiCo<sub>2</sub>O<sub>4</sub> nanorods demonstrated excellent electrochemical activity towards the electrooxidation of methanol with a high catalytic current density and long-term stability. Overall, the current investigation opens a new approach for the shape-controlled synthesis of a highly efficient non-noble electrocatalyst for methanol oxidation with high catalytic activity and stability.

Keywords: Methanol, Non-noble Metal, Nickel boride, CoS<sub>2</sub>/MoS<sub>2</sub>/rGO, NiCo<sub>2</sub>O<sub>4</sub> nanorod

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# Adsorptive stripping voltammetric assay of Octogen explosive on MWCNTs-Ag nanocomposite electrode

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Cyclotetramethylene-tetranitramine, commonly called Octogen or HMX, is one of the strongest military explosives, that due to its high detonation velocity and thermal stability, is used commonly in various energetic materials of ammunitions and rocket and missile warheads[1]. Octogen, having nitramine functional group, has a chemical behavior similar to its similar homologue cyclotrimethylenetrinitramine (RDX), but, unexpectedly, the reduction signal of HMX is very weak on the conventional electrodes [2], and the scientific reports about this compound are limited. The use of unique electrochemical methods, is an appropriate method for inexpensive and fast field detection of explosives. Here, an efficient electrocatalyst based on multi-walled carbon nanotubes-silver (MWCNTs)/Ag nanocomposite modified glassy carbon electrode (GCE) was developed by controlled electrodeposition and continuous double-potential pulses, to assay Octogen using voltammetric techniques. The electrochemical behavior of system in various pHs was studied and some reduction parameters such as the transfer coefficient ( $\alpha$ ), electron transfer number and apparent diffusion coefficient constant of Octogen were estimated. The results demonstrated that reduction of Octogen by adsorption stripping voltammetry on MWCNTs/Ag film can remarkably be enhanced and catalyzed compared to bare carbon nanotubes electrode, and the reduction potential facilities from -0.7 V (vs. SCE) to -0.3 V. Chronoamperometry studies show a diffusion-controlled process with apparent diffusion coefficient of  $2.01 \times 10^{-4}$  cm<sup>2</sup> s<sup>-1</sup>. Also, chronocoulometric studies show that the number of electrons transferred for electrochemical oxidation of Octogen are near to 1.98. Under optimized conditions, the reduction peak have two linear dynamic ranges of 2.0-30.0 and 30.0-120.0  $\Box$ M with the experimental detection limit of 0.2  $\Box$ M and a precision of <2.5% (RSD for 5 analysis). This modified electrode can be properly used for the determination of HMX in soil and ground water samples with satisfactory results. **REFERENCES:** 

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# A Comprehensive Study for Electrochemical Behavior of Hazardous Pesticide Fenitrothion in Aqueous Solutions

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Persistent organophosphorus (OPS) compounds are well-known toxic substances, which are used as pesticides, herbicides and insecticides agents [1]. The high toxicity of these compounds and their use in different activities such as agriculture increases public concerns. Fenitrothion (FT) is one of the organophosphate compounds that is widely used as a pesticide [2]. Because of the extensive use of this pesticide in agricultural areas, and the high persistence of these compounds the residue of these compounds remains in our environment and leads to allergies, respiratory problems, lung disease and a variety of cancers [3,4]. In this study, the electrochemical behavior of FT was investigated using cyclic voltammetry on the glassy carbon electrode. The effects of pH and potential scan rate on peak potential and peak current of redox couples (ArNHOH/ArNO) produced from the reduction of NO<sub>2</sub> group of FT were studied. Cyclic voltammograms of FT at various pH values indicated that the potential of anodic peak  $(E_{pA1})$  and its cathodic counterpart  $(E_{pC1})$  depend on the pH of the solution and shift to the negative values by increasing pH. This is due to the participation of proton(s) in the oxidation of FT red (ArNHOH) to FT<sub>ox</sub> (ArNO). The effect of potential sweep rate on the anodic and cathodic peak current of FT<sub>red</sub>/FT<sub>ox</sub> couple produced from the reduction of FT was studied on the GCE by cyclic voltammetry. The results showed that the anodic and cathodic peak current of  $FT_{red}/FT_{ox}$  couple vary linearly with the square root of scan rate (v<sup>1/2</sup>), which confirms the diffusion-controlled process for electrooxidation of FT<sub>red</sub> and reduction of FT<sub>ox</sub> on the surface of GCE at the studied potential scan rates. Finally based on the results, a reaction mechanism involving 4-electron/4-proton reduction of the nitro-functional group of FT and also two electron/two proton oxidation of FT<sub>red</sub> were proposed.



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## Electrochemical Behavior and Oxidation Mechanism of Hydroxychloroqui ne as aDrug Treating COVID-19 in Aqueous Solutions

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Hydroxychloroquine (HCQ), a derivative of 4-aminoquinolone, is pre-scribed as an antimalar ial prevention drug and to treat diseases such as rheumatoid arthritis, and systemic lupus eryth ematous [1]. Recently, international medical organizations over the world allowed the treatme nt of coronavirus (COVID-19) in certain hospitalized patients by chloroquine and hydroxychl oroquine [2,3]. Huge amounts of HCQ are needed for the treatment of different diseases inclu ding Covid-19 over the world. This certainly results in the discharge of large quantities of was tewaters contaminated with hydroxychloroquine into the environment. Due to its chemical an d biological properties, HCQ has a high potential to persist, bioaccumulate, and transfer to liv ing organisms in intensified toxic forms. The high risks of natural water contamination due to the large production and utilization of HCQ, necessitates more attention to limit its hazardous effects on human health and the environment [1-4]. In this study, the electrochemical behavio r and oxidation mechanism of HCQ as a drug treating COVID-19 in aqueous solutions was in vestigated using cyclic voltammetry on the glassy carbon electrode. The effects of pH and pot ential scan rate on peak potential and peak current of oxidation produced from the oxidation o f HCQ were studied. Cyclic voltammograms of HCQ at various pH values indicated that the p otential of anodic peak (EpA1) depends on the pH of the solution and shift to the negative val ues by increasing pH. This is due to the participation of proton(s) in the oxidation of HCQ to t he form of HCQ<sub>red</sub>. The results for the investigation of the effect of potential sweep rate on th

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e anodic peak current of HCQ on the GCE by cyclic voltammetry indicated that the anodic pe ak current is almost equal with the square root of scan rate ( $v^{1/2}$ ), this confirms that considering the anodic peak current and based on the Randles–Sevcik equation, the absorptive-controlled process for electrooxidation of HCQ on the surface of GCE [5]. According to the acquired pot ential-pH diagram and the oxidation of the HCQ, a reaction mechanism involving 1-electron/ 2-proton oxidation of HCQ was proposed. Finally,according to the results, our prediction for t he oxidation of HCQ is through the CE mechanism.

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# A Chemometric-Assisted Voltammetric Method for Simultaneous Determination of Acetaminophen and Diclofenac

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ABSTRACT: Diclofenac (DCF) and acetaminophen (ACT) are two of the most important nonsteroidal anti-inflammatory drugs due to their antipyretic, analgesic and anti-inflammatory properties [1]. Furthermore, ACT and DCF exhibit synergistic activity towards pain relief. Therefore analytical methods suitable for the simultaneous quantification of these NSAIDs in both urine and pharmaceuticals, are required [2]. In this study, a methodology for direct and simultaneous determination of acetaminophen and diclofenac using voltammetric method associated with the partial least squares (PLS) and genetic algorithm-partial least squares (GA-PLS) is presented. Here PLS regression methods are applied in voltammetric data collected by the previous developed voltammetric method aiming to combine the sensibility of pulse voltammetry (DPV) with the capacity PLS to resolve overlapped signals. The calibration set was based on the differential pulse voltammetry for 32 different mixtures of ACT and DCF. The calibration curve was linear over the concentration range of 0.1-100 and 100-1000 µL for ACT and DCF respectively. These two methods were tested by analyzing the synthetic mixtures of the ACT and DCF and they were applied to real samples containing a commercial pharmaceutical preparation of the subject drugs. Good results were obtained by the two methods. However, the accuracy of the GA-PLS method was better than that of the PLS method.

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## **Electrochemical Synthesis of New Organic Compound Based on The Oxidation of 4-tert-Butylcatechol in The Presence of Desloratadine**

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Organic electrosynthesis is synthesizing organic compounds by electricity. There are several merits rather than other methods that can encourage chemists to use organic electrosynthesis. For instance, under oxidant-free or reductant-free conditions and being environmentally friendly. Additionally compared to traditional methods that often proceed at elevated temperature or pressure, electrochemical reactions are usually carried out under milder conditions providing an energy-saving option. Nowadays, synthesizing new drug derivatives is one the most important issues. 8-chloro-11-(piperidin-4-ylidene)-6,11-dihydro-5Hbenzo[4,5]cyclohepta[2,1-b]pyridine (Desloratadine) is a drug belongs to antihistamines group which is used for allergy symptoms. It is a member of secondary amines and has a NH group in its structure which can operates as a nucleophile in Michael addition reaction for electrochemical synthesis. In this work, electrochemical oxidation of 4-tertiobutyl catechol has been studied in the presence of desloratadine as nucleophile in a mixture of ethanol/water solution by means of cyclic voltammetry as a diagnostic technique. The results indicate the participation of desloratadine in the Michael addition reaction with the oxidized form of 4tertiobutyl catechol as a Michael acceptor to produce new amino derivative via ECE mechanism. At the first, 4-tertiobutyl catechol oxidized (E) and produces guinone form to react with desloratadine and produces an intermediate (C), in continue the oxidation of this compound is easier than the oxidation of parent starting molecule by virtue of the presence of electron-donating group of secondary amine (E) to produce final product. Moreover, antibacterial properties of final product has been estimated. At the end, this final product has been characterized by cyclic voltammetry, IR, NMR and Mass spectroscopy. **REFERENCES:** 

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# Process Optimization and Degradation Pathway for Electrocatalytic Degradation of 2,4,6-Trinitrophenol by Graphite Modified Lead Dioxide Anode

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A novel idea for the electrochemical mineralization of environmentally persistent 2, 4, 6trinitrophenol (TNP) has been investigated in aqueous solutions on the Graphite/ $\beta$ -PbO<sub>2</sub> anode by electrocatalytic degradation method. This anode shows high overvoltage for oxygen evolution, long service lifetime and excellent electrocatalytic degradation efficiency for persistent organic pollutants. Subsequently, the surface morphology and crystal structure of the anode were characterized and identified by different techniques such as FESEM, EDX and XRD. The influence of several operating parameters, such as initial concentration TNP (50-100 mg L<sup>-1</sup>), applied current density (2-5 mA cm<sup>-2</sup>) and initial pH value (3.0, 7.0 and 10.0), kinetics, current efficiency and electrochemical energy consumption on the electrocatalytic degradation of TNP has been thoroughly examined. The results showed that the degradation of TNP reached up to 98% and COD removal up to 93% after 75 min electrolysis at the initial 50 mg  $L^{-1}$  TNP concentration, respectively. The electrochemical characteristics of the electrodes have been investigated by LSV and CV, results show that electrodeposition of  $\beta$ -PbO<sub>2</sub> on the graphite lead to high overpotential for OER in this electrode, more stability and lifetime electrode. As a significant consequence, results showed that the TNP degradation process on this electrode leads to the reduction of the TNP to its amine form on the cathode surface, and then the attack of hydroxyl radicals electrogenerated (•OH) on the anodic material, the opening of aromatic rings and finally oxidized into CO<sub>2</sub> and H<sub>2</sub>O on the anode surface. Kinetic studies indicated that the electrocatalytic degradation of TNP on the graphite/β–PbO<sub>2</sub> electrode followed pseudo-first-order reaction. This study demonstrates an unusual route

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through a new concept for electrocatalytic degradation method in the removal of nitroaromatic compounds. We also proposed the degradation mechanism and mineralization pathway of TNP on graphite/ $\beta$ -PbO<sub>2</sub> electrode.

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# Electrochemical Dimerization of 4-phenylhydrazinsulfonamide hydrochloride

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Azo dyes are an important class of organic compounds contributing an impressive range of colors. They can tautomerize to azohydrazone, azo-imino, and azonium/ammonium. They are widelyused as colorants in the different products, for example paper, textiles, foodstuffs, leather and gasoline. Azo dyes are made by diazotization of a primary aromatic amine and reaction of generated diazonium salt with a nucleophile (electron-rich), rhodium-catalyzed regioselective C–N bond formation with azides, oxidative dimerization of aromatic amines using tert-butyl hypoiodite (t-BuOI) and redox-driven C-N bond fusion. However, these methods have the disadvantages such as strongly acidic and/or basic media, tedious work-up, heavy metal pollution and safety problems.

Electrochemistry has emerged as a powerful tool for the synthesis of complex organic molecules in green condition. These disadvantages have encouraged us to develop an eco-friendly procedure for the synthesis of new azo dye using electrochemical oxidation of 4-phenylhydrazinsulfonamide hydrochloride. The main objective of this paper is to present a facile and one-pot electrochemical process under mild conditions at a carbon electrode, using an environmentally friendly method for the synthesis of new azo compound.

On the other hand, 4-phenylhydrazinsulfonamide hydrochloride is a phenylhydrazine derivative with good biological properties. Phenylhydrazines are an important group of organic



compounds with the chemical formula  $C_6H_5NHNH_2$ . Phenylhydrazine is prepared by oxidizing aniline with sodium nitrite in the presence of hydrogen chloride to form the diazonium salt, which is then reduced using sodium sulfite in the presence of sodium hydroxide to form the final product.

In this work, two main objectives were pursued. (1) electrochemical oxidation of 4phenylhydrazinsulfonamide hydrochloride at various pH and depicting of E-pH diagram for calculation of number of electrons and protons during oxidation process. (2) the synthesis of new azo compound via constant current electrolysis in green media. The azo dye has been characterized via some spectral data such as MS, FT-IR, and NMR.

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# Electrochemical Generation of Aryl Diazonium and Polymerization by Radical Initiator, Electropolymerization and Characterization of Acrylic Acid

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The electrochemical report for aryl diazonium cation generation from nitro arenes in two-phase (ethyl acetate/water) and one-pot was reported in this work. Electroconversion of nitroarene to related aniline at carbon electrode surface in ethyl acetate phase was done successfully by using perchloric acid as proton source and supporting electrolyte. By generation of diazonium cation in water phase, in the next step, by using copper rod as anode in water phase, novel and facile strategy for copper (I) cation generation in water phase, as well as a radical Initiator was stablished for polymerization reactions. This novel strategy led us to using nitro arenes for facile polymerization of AA without using any organic or inorganic catalyst or high temperature. The preparation of poly(acrylic acid) (PAA) with tailored architecture and morphology is important for the design of advanced polymer materials. In this study, a green and simple strategy for the electropolymerization of AA is developed. Our data show that the polymerization of acrylic acid creates an attractive architecture of an insulating porosity-free film on the electrode. The electropolymerization process is performed without the need for any pretreatment or change of substrate in water and room temperature. The structural properties and final characteristics in respect of adhesion and the barrier coating of the resulting deposited coatings were investigated by means of the fourier transform infrared spectroscopy (FT-IR), field emission scanning electron microscopy (FE-SEM), energy dispersive X-ray analysis (EDX), mapping analysis, transmission Electron Microscopy (TEM), x-ray diffraction analysis (XRD), gel permeation chromatography (GPC), thermal gravimetric analysis (TGA) and derivative thermogravimetry (DTG). The electrochemical performance of the modified


electrode is also evaluated by cyclic voltammetry and electrochemical impedance spectroscopy.

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## Determination of the herbicide paraquat using the new Ag-GO/CuO/GCE modified glassy carbon electrode by DPV

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Finding the synergistic electrochemical effect of cuprous oxide nanoparticle (CuO-NP), Agnanoparticle (Ag-NP) on graphene oxide (GO) encouraged us to provide a novel modified glassy carbon electrode (GCE) for the determination of the herbicide parquet (PQ) in solution. The bank compounds were prepared by simple methods and characterized by scanning electronic microscopy (SEM), UV/Vis spectroscopy, and electrochemical impedance spectroscopy (EIS). Electrochemical measurements were investigated by Differential Pulse Voltammetry (DPV). The sensor showed good electrocatalytic activity towards the reduction of PQ. The Cyclic Voltammetric (CV) and DPV results showed that the oxidation and reduction process of PQ is reversible and the Ag-GO/CuO composition had good electrocatalytic performances in the determination of PQ. The responses of the electrochemical Ag-GO/CuO/GCE were investigated for pH, type of supporting electrolyte, scan rate, and the response reproducibility of the system. Under the optimized conditions, a linear response over the concentration range of 0.40-650.0  $\mu$ M of PQ was observed with a correlation coefficient (R2) of 0.999 and a detection limit (LOD) of 0.07  $\mu$ M. Reasonable recoveries between 99.2 to 105.0% were obtained for river water PQ content.

Keywords: cuprous oxide nanoparticle; graphene oxide; paraquat; silver nanoparticle



## Electrochemical Determination of Diclofenac Using a Pencil Graphite Electrode Modified With Halloysite Capped Gold– Palladium Bimetallic Nanoparticles

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Diclofenac sodium is a nonsteroidal drug with the analgesic, anti-inflammatory and antipyretic properties [1]. It may have adverse effects on human body such as anemia; disorder in gastrointestinal function and renal disorders [2]. Therefore, it is necessary to determine the concentration of diclofenac in pharmaceutical and biological samples. Among different analytical methods, the electrochemical techniques are suitable for quantification of diclofenac in solutions. In this research project, a simple, low cost and sensitive electrochemical sensor was fabricated at the surface of pencil graphite electrode (PGE) for determination of diclofenac through layer by layer modification of halloysite film and gold-palladium bimetallic nanoparticles. Halloysite was introduced to increase the specific surface area of the pencil graphite electrode. The PGE electrode was immersed in a 1 mgr ml<sup>-1</sup> halloysite suspension for 24 h and the solvent was evaporated using an infrared lamp. Electrochemical deposition method was employed for immobilization of gold-palladium nanoparticles at the surface of halloysite modified electrode. The surface morphology of the pencil graphite electrode was investigated by scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS) techniques at each modification step. Cyclic voltammetry (CV) was used to characterize the electrochemical behavior of diclofenac molecules. The effect of halloysite amount, number of scan cycles of electrodeposition of gold-palladium nanoparticles and pH on the analytical performance of the proposed sensor was investigated. The influence of interfering species such as citric acid, uric acid, ascorbic acid and glucose was evaluated and the results showed that the developed sensor has a high selectivity toward diclofenac molecules. Also, the proposed electrochemical sensor, showed a low detection limit, wide linear range and a good stability, repeatability and reproducibility for diclofenac determination in solutions. Moreover, the prepared sensor was successfully employed for determination the low concentration of diclofenac in real samples with satisfactory results.

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## Electrocatalytic oxidation and determination of paractamole onto functionalized reduced graphene oxide: electrochemical and computational study

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Improving the sensivity, lowering the determination limit and promoting the response rate are important for analytical determination of biological, pharmaceutical, and environmental research. The sensitivity may be improved by incorporation of a substrate-recycling schem [1,2] and several strategies including catalysts, enzymes, mediators, and mesoporous materials. Electrochemical analysis has attracted considerable attention because it can analyze not only the electro-active materials.

In this study, the electrocatalytic oxidation of paractamole was investigated on a functionalized graphene modified graphite electrode. The oxidation process involved and its kinetics were investigated using cyclic voltammetry, chronoamperometry, and electrochemical impedance spectroscopy techniques, as well as steady-state polarization measurements. The rate constants of the catalytic oxidation of the drugs and the electron-transfer coefficients are reported. A sensitive, simple, and time-saving amperometric procedure was developed for the analysis of pareactamole, with detection limits of 20  $\mu$ M. The electrode was used for the direct assay of paractamol tablet. Also, using AIM2000 software, electron energy, electron density, Lagrangian kinetic energy, Hamiltonian kinetic energy density, electron kinetic energy, charge and Laplace electron density were calculated and investigated for different atomic substrates in this study.

Keywords:Paractamol, computational, Electrochemical, paractamole

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## High Performance Electrocatalyst for Electrocatalysis of Oxygen Reduction Reaction by Carbonized ZIF-67 Support

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Pt and Pt-based catalysts were demonstrated to be high-performance electrocatalysts for ORR in the PEMFCs [1]. Due to the high cost and scarcity of Pt; large-scale practical applications are significantly limited [2]. Researchers have made the Pt-M (M = Co, Ni, Cu, Cr, Fe, etc.) bimetallic catalyst to reduce the Pt usage and increase activity of Pt catalysts [3]. Also, support materials reduce the amount of Pt loading, prevents the accumulation of Pt nanoparticles and increase ORR performance due to porosity, high surface area, electrical conductivity and corrosion resistance [4]. In this study, Pt/Co bimetallic nanoparticles supported nanoporous carbon composite (Pt/Co-NC) were prepared as a new type of high-performance electrocatalysts for oxygen reduction reaction (ORR). This composite is synthesized by two steps procedure involving preparation of Co-NC according to templating method through direct carbonization of zeolitic imidazolate framework 67 (ZIF-67) as a template in N<sub>2</sub> atmosphere at 900 °C. This procedure is followed by partial galvanic replacement of Co metals by Pt (IV) ions, upon immersion in K<sub>2</sub>PtCl<sub>6</sub> (1.5 mM) solution. Co-NC support plays a key role for Pt catalyst performance. Pt/Co-NC is tested for the ORR performance in 2 M H<sub>2</sub>SO<sub>4</sub> solution in the cathodic half-cell. The polarization curves have shown that the Pt/Co-NC exhibit higher current density and superior power density rather than the Pt/C. This is attributed to synergetic effect of the Pt-Co bimetallic catalyst and uniform distribution of the Pt nanoparticles at the support surface.

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## The Electrochemical Study of Hydroquinone in The Presence of 2-Amino-5-mercapto-1,3,4-thiadiazole as Nucleophile: a Green Strategy to Synthesis a Novel Thiadiazole Derivative

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Electroorganic synthesis has considered as a valuable-powerful method for the development of environmentally friendly processes in the recent decades, this conception is because of lowenergy consumption and temperature, high selectivity, good atom economy, low costs for reagents, and moreover, electrons are considering as clean reagents too. Hydroquinone (HQ) is a natural ingredient in many agricultural products, such as vegetables, fruits and grains which is widely using as a reducing agent, antioxidant, polymerization inhibitor and also over-thecounter drugs such as skin lighteners. The p-benzoquinone which is the oxidized form of HQ is very reactive and can be attacked by variety of nucleophiles. Generally 1,3,4-thiadiazole derivatives are the well-known five-membered heterocycles which displaying a broad spectrum of biological activities such as antioxidant, antimicrobial, anti-inflammatory, antituberculosis, anticonvulsants, and anxiolytic. The focus of this study is on 2-Amino-5-mercapto-1,3,4-thiadiazole (AMT) which is a highly reactive molecule. The nucleophilic property of AMT which resulted from two active groups of amine and thiol made us to involve it in a Michael I 4<sup>th</sup> Biennial Electrochemistry Seminar of IRAN August 2021



addition reaction with p-benzoquinone, the unique structure of AMT is also shows a dual behavior as both nucleophile and substrate. Therefore the electrochemical dimerization mechanism of AMT had also studied, In the following, the electrochemical behavior of HQ in the presence of AMT as nucleophile has been investigated by cyclic voltammetry technique in different aqueous buffer solutions (pH=4.00-8.00, c=0.2 M). The voltammograms showed an anodic peak (a<sub>1</sub>) and its corresponding cathodic peak (c<sub>1</sub>) and also a single cathodic peak (c<sub>2</sub>) which based on an EC mechanism. Subsequently Controlled-potential-coulometry (CPC) and Constant-current-coulometry (CCC) methods were used under a series of optimization (one factor at the time technique) for high yield synthesis of products under mild experimental conditions and the obtained powders were characterized perfectly via: FT-IR, 1H-NMR, 13C-NMR and MS.

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### **Electrochemical Behavior of 1-(4-Nitrophenyl) Piperazin**

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Electrochemical synthesis is a well-established method for the synthesis of organic compounds. The most important advantages of electrochemical methods over conventional synthesis methods are the ability to carry out the reaction under mild conditions, the lack of a need for additional chemical reagents such as oxidizing or reducing agents, the easy scalability, and the environmental friendliness. Nitro compounds are an important class of organic compounds in the synthesis of organic chemistry. They are widely used as chemicals in the manufacture of medicines, explosives, paints, fertilizers, plastics and perfumes. The reduction of the nitro group represents a powerful and widely used transformation that allows to introducing variety of functional groups in the molecule. To evaluate the usability of the method, we have investigated the electrochemical behavior of 1-(4-Nitrophenyl) Piperazin (4NP) via cyclic voltammetry. 4NP is a highly polar substance that dissolves well in polar solvents such as ethanol, methanol, acetone and etc. In the first step, the study of 4NP was performed at different pH (1.0-10.0) and scan rates (10, 25, 50, 100, 500 and 1000 mv/s) in water/ethanol (70/30 v/v) mixture. The effect of pH on the cyclic voltammetric response of 4NP has been examined. The data show that the potential of all three peaks (A<sub>1</sub>, C<sub>1</sub>, A<sub>2</sub>, C<sub>2</sub> and C<sub>0</sub>) are pH-dependent. By depicting of pourbaix diagram, the number of electrons and protons were achieved. By scanning the electrode potential from -0.30 V to a sufficiently negative voltage (-0.95 V) (curve b), the cyclic voltammogram exhibits a large irreversible cathodic peak  $(C_0)$ corresponding to the reduction of 4NP to hydroxylamine (PHA) form and two reversible redox system  $(A_1/C_1 \text{ and } A_2/C_2)$  ascribed to the redox couple hydroxylamine/nitrosobenzene (PHA/NSB) and oxidation of benzene ring, respectively. An important feature of the peaks

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current ratio,  $I_{pA1}/I_{pC1}$  and  $I_{pA2}/I_{pC2}$  is that the current ratio is depends on the potential scan rate, as, with increasing potential scan rate,  $I_{pA1}/I_{pC1}$  and  $I_{pA2}/I_{pC2}$  increases. In this work, diffusion coefficient of 4NP were determined via chronoamperometry technique.

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## Synthesis and characterization of new metal oxides nanostructures for ozone generation with high-efficiency electrochemical method

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Ozone is a strong oxidant with the oxidation-reduction potential (ORP) about 2.07 V, which is higher than that of hydrogen peroxides (1.77V) and chlorine (1.36V). Ozone is an environmentally- friendly oxidant that is widely used for industrial applications, such as water disinfection, air purification, and medical use. Electrochemical ozone production (EOP) can provide very high concentrations of the reagent in both the gas phase and solution[1]. The electrolysis of water is generally believed to generate ozone by a six-electron reaction (Eq. 1):

$$3H_2O \rightarrow O_3 + 6H^+ + 6e^- E^\circ = 1.56V \text{ vs RHE}$$
 (1)

Whiles, E0 for the four-electron process of water oxidation to produce oxygen is somewhat lower(Eq.2)

$$2H_2O \rightarrow O_2 + 4H^+ + 4e^- E^\circ = 1.23V \text{ vs RHE}$$
 (2)

Thus, the producing-oxygen from water always take place with ozone generation, therefore the current efficiency for ozone generation is the percentage of the observed current [2]. Accordingly, minimizing oxygen evolution reaction) OER (is a key requirement for EOP with an appropriate current efficiency. Under electrolysis condition, effective approaches should be developed to substantially increase the overpotential of the OER, to prohibit the competitive oxygen generation [3]. This approach can be achieved by suitable choice of the anode material to have a high overpotential for OER. In addition to, the material electrode in anode should have good conductance, high durability under drastic operating conditions, and particularly good electrocatalytic activity for ozone production. Different electrodes contain β-PbO2, Pt, Pt composites, boron-doped diamond, TiO2 thin films on Si/TiOx/Pt substrate, and Ti/Ni-Sb-SnO2 catalysts are among the materials that have been used for EOP. [1-5] In this work, a highperformance porous titanium oxide electrode (Ti/TiO2/ Ni-Sb-SnO2) has been developed for electrochemical production of ozone(Fig. 1 a). The Ti/TiO2 electrode was prepared using anodizing method at high voltage for forming a layer of porous TiO2 on the surface of Ti mesh, then followed by depositing a layer of Ni-Sb-SnO2 under deep eutectic solvent on the Ti/TiO2 surface The deep eutectic solvent was used for electrodepositing, because its great effect on electrode performance. The conventional electrodes prepared by electrodepositing in aqueous solvent has poor electrochemical activity and short service life. The enhance properties can be related due to increase electrochemically active surface area of electrode which has a higher roughness, multilayer and uniform surface with pack structure of nanoparticles. Moreover, this electrode has good optical activity (Fig. 1 b) Ozone was electrogenerated from HClO4 solutions on Ti/TiO2/ Ni-Sb-SnO2 electrodes at different operating conditions. Higher



efficiency of O3 generation was obtained at 2.8 V in 1 M HClO4 (Fig. 1 c). Finally, The result of electrochemically

and morphologically characterization of prepared electrodes by linear sweep voltammetry and scanning electron microscopy(SEM) showed that the electrodes were efficient for EOP.



Fig. 1: (a) SEM morphologies of the Ti/TiO2/ Ni-Sb-SnO2 anode, (b) Anodic linear sweeps at a scan rate of 50 mV/s in 1 M HClO4 at 25°0C E (V) vs. Ag/AgCl/KCl (sat.), and (c) Optical activity of the anode in chronoamperometry.

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### Electrochemical Study of 2,4-Dinitrophenylhydrazine

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Electrochemistry is defined as the branch of chemistry that examines the phenomena resulting from combined chemical and electrical effects Electrochemical methods were considered due to their high sensitivity, higher efficiency, selectivity, separation and purification. Organic electrochemistry is concerned with the reduction and oxidation of organic molecules at the surface of electrodes. The electrochemical reduction of nitro compounds played an important role in the development of organic electrochemistry.

Compounds which containing Nitro groups are valuable building blocks because of their convenient transformation into a wide variety of synthetically important compounds such as amines, carboxylic acids, aldehydes, and nitriles. The nitro group is one of the most versatile and useful functional groups in organic synthesis and is an excellent electron acceptor. The reduction of polynitroaromatic compounds is complicated by multi-step processes. 2,4-Dinitrophenylhydrazine (DNPH) is a mutagenic agent and is commonly used as a reagent for the detection of aldehydes and ketones. DNPH contains three main functional groups that can oxidized and reduced at the surface glassy carbon electrode. Two nitro group in m-position and, hydrazine moiety (NH-NH<sub>2</sub>). Based these data, DNPH is a three functional molecule that indicate an interest voltametric shape. In negative-going scan, the nitro groups can individually reduced and indicated two reduction peaks. In positive-going scan, the hydarin moiety is oxidized to N=NH functional group. In this study, a comprehensive electrochemical behavior of DNPH has been performed via cyclic voltammetry and chronoamperometry techniques. At first, electrochemival study of DNPH was carried out in different pH and green condition. All

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of reduction and oxidation peaks are shifted to negative value with increasing basic media. In following, the number of electrons and protons were calculated via pourbiax diagram (E-pH). For more data, diffusion coefficient of DNPH was obtained with chronoamperometry method.

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## A Green Strategy for The Synthesis of Fluorinated Derivatives of p-Methylaminophenol

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Electrochemical redox reactions produce highly reactive intermediates, such as: anions, cations, radical ions, radicals, and nucleophilic as well as electrophilic groups. The controllable electron transfer process causes to change the electron-poor and electrophilic character of a functional group to be nucleophilic or vice versa. Between electrochemical functionalization process, fluorination is a favorable reaction and have no negative conditions such as using catalyst, high temperature and pressure. These data promoted us to use batch electrochemical cell for fluorination of relevant compounds. Among the electrochemical techniques, cyclic voltammetry is a popular technique which is used for electrochemical studies of electrode processes. Aminophenol derivatives have attracted scientific interest in both chemical and electrochemical studies. A wide range of pharmacological activities have been reported for p-aminophenol and related molecules. Many aminophenol derivatives are known to be effective antioxidants and to be capable of modifying the direction of various freeradical processes. These compounds are important intermediates for the manufacture products and drug industries. In this work, the electrochemical oxidation of p-methylaminophenol in the presence of tetrabutylammonium fluoride as a fluorine source has been investigated in non-buffered solution. Based on literature review, many researchers applied tetrabutylammonium fluoride for electrofluorination of organic compounds in non-aqueous solution. The voltammetric study confirms that the electrogenerated p-methylquinoneimine can be reacted with F- and produce of fluorinated derivatives of pmethylaminophenol. Based on the results which obtained from the voltammetric data, the micro scale electrolysis was performed under the constant current method in order to synthesis of new product. After the electrolysis process, the fluorinated derivative of p-methylaminophenol was purified by the thin layer chromatography and characterized by FT-IR, H-NMR, MS.



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## Electrochemiluminescence-based Nanozyme for Prostate-Specific Antigen using the Luminol-loaded Graphitic Carbon Nitride Nanosheets (C<sub>3</sub>N<sub>4</sub> NS)encapsulated NH<sub>2</sub>-MIL(53)-Fe

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Developing sensitive strategies to detect the biomarkers is responsible for early detection of a genetic disorder and cancer-related biomarkers. Artificial enzymes based on nanomaterial (nanozymes), in contrast to natural enzymes, have recently attracted much more attention due to the superior advantages, such as high durability, simple preparation, tunable catalytic activities, and low-cost .The function of separating nanozymes, resulted in decreased local concentrations of i.e., nanozymes and their intermediate products such as O<sub>2</sub>, hydroxyl (\*OH) and hydroperoxyl (\*OOH) radicals, limiting overall effectiveness of the enzymatic mimic processes. One technique aimed at overcoming these limitations is to confine the nanozymes within a protective coating such as metal-organic frameworks (MOFs).

Electrochemiluminescence-based methods, owing to the lack of a required external light source, and consequently, no scattering and excitation source fluctuations, resulted in to improve detection limit and sensitivity .Herein, a rational design of high catalytic activity of artificial enzyme mimics with enhancing the robustness of functional nanozymes has been introduced to detect PSA as a model target. Using a separation/enrichment tool of capture antibody (cAb1)-modified magnetic nanoparticles (MNPs/cAb1), signal amplifier luminol (LUM)-loaded graphitic carbon nitride nanosheets (C<sub>3</sub>N<sub>4</sub> NS)-encapsulated NH<sub>2</sub>-MIL(53)-Fe (NMF) (C<sub>3</sub>N<sub>4</sub>@LUM/NMF)) to label signal antibody (Ab2) as a specific targeting and a supporting platform of a nanoporous gold electrode (NPGE) with high-efficiency electron acceleration, a cascade signal amplification strategy has been achieved. In addition, the

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nanoscale proximity effect of confined LUM within the  $C_3N_4@NMF$  nanozyme and synergistically enhanced catalytic activity causes significantly to promote the ECL of LUM owing to minimize the decomposition of highly active intermediates of •OH-generating reaction of  $C_3N_4@NMF$  nanozymes from  $H_2O_2$ . Taking the advantages of multipleamplification, the present strategy shows PSA detection in dynamic range of 0.1 pg mL<sup>-1</sup>-60 ng mL<sup>-1</sup> with 0.02 pg mL<sup>-1</sup> limit of detection. This ECL-based nanozyme opens a new horizon for high sensitive targeted bioanalysis with functional nanomaterial design.

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# Part 3

- Electrochemical Energy
- Generation & Storage
- Industrial Electrolysis
- Electrochemical Approaches to Renewable Energy
- Corrosion & Plating



## Coating the Negative Electrode Surface of Lead Acid Battery with a Layer of Carbon Composite for the Purpose of Ultrabattery Design

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There is growing demand for batteries that able to be recharged efficiently at high rate in car industry. A high rate of recharging of the battery is needed to associate with regenerative braking, which is required for good fuel economy in micro-hybrid electric vehicles. In lead-acid batteries used in this application, failure of the battery tended to occur at the negative plate, as a result of progressive accumulation of lead sulphate on the surfaces of the negative plates. This occurs because the lead sulphate cannot be converted efficiently back to sponge lead during high rate recharging. In this work we designed negative electrodes for ultrabattery by pasting a layer of carbon composite on conventional negative electrodes. The carbon composite including activated carbon, carbon black, graphite, and a binder. The weight percentage of the carbon composite layer is 3 % of total weight of the negative material. The plates cured, dried and formed according to conventional methods. Cycle life of the designed negative electrode (Neg. ultrabattery) and conventional negative electrode were tested according to the standard test method [1]. The results shows a threefold improvement in cycle life of the Neg. ultrabattery, under high rate partial state of charge (HRPSoC) conditions.

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## Preparation of vanadium-copper nanocomposite as a nanocatalyst anchored on carbon nanofibers to modification of cathode and improvement in rechargeable Li-CO<sub>2</sub> batteries performance

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Conversion of CO<sub>2</sub> as green-house gas to electrical energy has been considered for most researchers as essential approach for mitigating climate changes and achieving sustainable development. In recent years, various routes have been investigated to fulfill this purpose. Lithium-carbon dioxide (Li-CO<sub>2</sub>) batteries well known as one kinds of novel and innovational technique/device that could coinstantaneous capture and convert carbon dioxide to electrical energy and then differing from traditionally electrochemical devices. Rechargeable lithiumcarbon dioxide is attracting increasing attention due to their high energy density and ability to capture greenhouse gas CO<sub>2</sub>. However, the difficulty in decomposing electronically insulating and electrochemically sluggish Li<sub>2</sub>CO<sub>3</sub> as discharge product under low charge potential is still a major challenge in these batteries. The work principle of lithium-carbon dioxide batteries was proposed to comply with reversibly electrochemical reaction of  $4\text{Li}+3\text{CO}_2\leftrightarrow 2\text{Li}_2\text{CO}_3+\text{C}$ , which could theoretically deliver a high energy density of 1876 Wh/kg. However, Li<sub>2</sub>CO<sub>3</sub>, as the main discharge product, is much thermodynamically stable, electronically insulating and electrochemically sluggish. As a result, the difficulty of completely electrochemical decomposition of Li<sub>2</sub>CO<sub>3</sub> within a low potential during the charge process seriously lowers energy efficiency and hinders more deployment of these batteries. Based on the several results of researches to solve of this problem, it's found that electrocatalysts utilized such as carbon nanomaterials, transition metals, metal oxides, metal carbides and redox mediator could be facilitate the kinetics of discharge and charge processes in lithium-carbon dioxide batteries. In I 4<sup>th</sup> Biennial Electrochemistry Seminar of IRAN August 2021



present work, a composite of vanadium-copper alloy with size of nanoparticles uniformly anchored on carbon nanofibers (V-Cu/CNFs) as an efficient cathode electrocatalyst for lithium-carbon dioxide batteries is well prepared. Obviously, based on the obtained results, the lithium-carbon dioxide batteries with V-Cu/CNFs cathodes can be steadily cycled for over 140 cycles without decreasing in the capacity. And it shows record-high rate capability along with much decreased over-potential of 1.35 at current density of 1000 mA/g. Furthermore, a high discharge capacity of 11257 mAh/g is obtained and about 98.5% of discharged capacity could be reversibly charged. The results demonstrate the powerfully catalytic activity of intermixed V-Cu nanocomposite for easily decomposing discharge product in lithium-carbon dioxide batteries (i.e Li<sub>2</sub>CO<sub>3</sub>) and provides more insights to design more highly efficient cathode electrocatalysts for lithium-carbon dioxide batteries and beyond.

**Keywords**: Li-CO<sub>2</sub> rechargeable batteries, V-Cu nanocomposite, modification of cathode, improvement performance

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## Hydrothermal Assisted Formation of Cu<sub>2</sub>SnO<sub>4</sub> Nanoparticles as a High-Performance Electrode Material for Supercapacitors

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In recent years, supercapacitors have attracted significant attention due to the fast chargedischarge ability, excellent rate capability and long-time stability. In this study, for the first time, copper stannate nanoparticles (Cu<sub>2</sub>SnO<sub>4</sub> NPs) grown radially on nickel foam (NF) have been successfully constructed by a facile and cost-effective hydrothermal method. The physicochemical characteristics of the material were investigated by various techniques such as energy dispersive X-ray analysis (XRD), field-emission scanning electron microscopy (FESEM), and transmission electron microscopy (TEM). The Cu<sub>2</sub>SnO<sub>4</sub> nanoparticles were used as the active electrode material for supercapacitor applications. The electrochemical properties of the Cu<sub>2</sub>SnO<sub>4</sub> NPs as binder-free electrode for supercapacitor was examined by cyclic voltammetry (CV), galvanostatic charge and discharge analysis (GCD), electrochemical impedance spectroscopy (EIS), and cycle life measurements in 2 M KOH electrolyte. The GCD analysis exhibited a specific capacitance as high as 2329.68 F  $g^{-1}$  at 1 A  $g^{-1}$  and good rate capability (1330 F g<sup>-1</sup> at 70 A g<sup>-1</sup>) in a 2 M KOH electrolyte. This capacitor electrode has excellent cyclic stability with 91.40% capacitance retention after 3000 cycles at 20 A  $g^{-1}$ , together with 99.17% coulomb efficiency in three-electrode system. These excellent properties make Cu<sub>2</sub>SnO<sub>4</sub> NPs a promising electrode material for applications in renewable energy storage and open up great opportunities for supercapacitors in the future.

**Keywords:** Cu<sub>2</sub>SnO<sub>4</sub> nanoparticles; Supercapacitor; Hydrothermal method; Energy storage; Binary transition metal oxides

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## A Carbon Sandwich Anode With FeS<sub>2</sub> Decorated S, N Co-doped Graphene Quantum Dots For High Performance Microbial Fuel Cells

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Microbial fuel cells, which generate electricity based on metabolism of organic compounds by electrochemically active microorganisms, have received great attention worldwide due to their potential in recovering electrical energy from waste and inexhaustible biomass. Unfortunately, the difficulty of achieving the high power, especially in real samples, remains a bottleneck for their practical applications.

The performance of microbial fuel cells relies critically on extracellular electron transfer between intracellular respiratory chains of electrochemically active bacteria and extracellular anodes, which requires an electrochemically active biofilm that attaches to the anode surface and electron transfer mediators such as c-type cytochromes in electrochemically active bacteria. For the further enhancing performance of microbial fuel cells, it is essential to develop suitable anode materials, which are required with various characters, such as large surface area, excellent electronic conductivity, and high electrocatalytic activity towards electron transfer mediators.

Herein, S, N co-doped graphene quantum dots (S, N GQDs) decorated with ferrous disulfide (FeS<sub>2</sub>) (FeS<sub>2</sub>–S, N GQDs), are synthesized via a simple hydrothermal reaction, for the performance improvement of microbial fuel cell based on a mixed bacterial culture. Electrochemical measurements demonstrate that the as-synthesized FeS<sub>2</sub>–S, N GQDs exhibits excellent electrocatalytic activity for the charge transfer on anode, providing the cell with a maximum power density of 1128 mW m<sup>-2</sup>, which is strikingly higher than the bare carbon cloth anode (265)

mW m<sup>-2</sup>). The excellent performance of FeS<sub>2</sub>–S, N GQDs is ascribed to the increased electronic conductivity of bare carbon cloth by S, N GQDs and the high ability of FeS<sub>2</sub> to enrich electroactive bacteria, as demonstrated by high-throughput sequencing. Based on superior biocompatibility, low cost, environment-friendliness, and facile fabrication, the proposed



FeS<sub>2</sub>–S, N GQDs bioanode could have a great potential for high-performance and costeffective sustainable microbial fuel cells.

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# Investigation the effect of acid content of positive active material on the characterizations of lead acid battery

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Adding acid to the lead acid battery paste lead to forming different kind of lead sulfate structures that influence the performance of lead acid battery. In this investigation positive paste preparation is carried out with different ratio of acid/lead oxide. Positive active material was characterized by x-ray diffraction, SEM, BET and porosimetry analyses. Result shows that increasing the ratio of acid/lead oxide lead to increase the porosity of positive active material. Capacity of positive active material was measured according to  $C_{20}$ ,  $C_{10}$  and  $C_5$ . Result shows that increasing the ratio of acid/lead oxide lead to increase C20 capacity and decrease of C5 capacity. And finally cycle life of positive active material was investigated.

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## Electrodeposition of Ni-Fe on graphite rod as an efficient and binder-free electrocatalyst for overall water splitting

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The usage of active electrocatalysts is a useful approach to accelerate the kinetics of electrochemical reactions and to enhance the efficiency of water splitting. The purpose of this study is to use the cyclic voltammetry technique for electrodeposition of Ni-Fe on a graphite rod substrate as an active electrocatalyst for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). In this research, innovation in the synthesis of Ni-Fe electrocatalyst is done using cyclic voltammetry, and some important factors such as the range of applied potential, the scan rate, and the number of cycles are optimized. In addition, the used substrate is a graphite rod, which is cheap, stable, and has good electrical conductivity. The main results show that the optimized Ni-Fe coating on graphite rod substrate has promising HER activity with low overpotentials of -193.9, -394, and -687.3 mV at the current densities of -10, -100, and -400 mA. cm<sup>-2</sup>, respectively. Besides, the manufactured Ni-Fe electrocatalyst is extremely active toward OER, needing overpotentials of only 284 mV for 10 mA. cm<sup>-2</sup> current density. This study offers a method for generating an electrocatalyst that is a highly active, bifunctional, and binder-free electrocatalyst for water splitting that is both affordable and fast. As a result of

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these findings, this electrocatalyst appears to be the potential for creating renewable and green energy in industrial applications.

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## Synthesis of Organic Inorganic Hybrid Coating Containing SiO<sub>2</sub> Nanoparticles Via Sol-Gel Process

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In this work, the sol-gel process due to its properties such as low synthesis temperature, ability to control the surface profile and the shape of hybrids, abundance of precursors, less energy consumption, no requirement for expensive equipment, lower cost and being eco-friendly has been employed to synthesize an organic inorganic hybrid coating based on tetraethyl orthosilicate (TEOS) covalently bonded to epoxy resin through the coupling agent 3aminopropyl triethoxysilane (APTES). After synthesis of organic inorganic hybrid coating, SiO<sub>2</sub> nanoparticles were added to the hybrid structure. The prepared organic inorganic hybrid was coated on the surface of 304 stainless steel by spin coating technique and then left for 8 hours at room temperature (aging) and cured in oven at 60 °C for 6 hours to ensure complete curing. In the next step, potentiodynamic polarization test was conducted to evaluate the corrosion resistance properties of the hybrid coating after 30 hours immersion in 3.5% NaCl solution. It is generally known that higher E<sub>corr</sub> and lower i<sub>corr</sub> of the polarization curves indicate better corrosion protection. Since the Tafel curve of hybrid coating shifted to the positive direction compared with the untreated substrate, implying that the coating as a shield could effectively restrain the corrosion of 304 stainless steel. The E<sub>corr</sub> of hybrid coating is -0.347 V, which is more positive than that of the bare 304 stainless steel (-0.671 V). Moreover, the icorr of the hybrid coating  $(7.61 \times 10^{-9} \text{ A.cm}^{-2})$  is 2 orders of magnitude lower than that of the untreated substrate  $(2.16 \times 10^{-7} \text{ A.cm}^{-2})$ .



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## **Corrosion Protection Coating Using Commercial Epoxy Resin**

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The aim of the present study was to synthesize and preparation of an organic inorganic hybrid coating to protect 304 stainless steel against corrosion, which was accomplished by using tetraethyl orthosilicate (TEOS) as inorganic part, 3-aminopropyltriethoxysilane (APTES) as coupling agent and commercial epoxy resin as organic phase. The mentioned precursors were employed to synthesize hybrid coating via sol-gel method and then, the prepared hybrid film was coated on the surface of 304 stainless steel by dip coating technique. After coating process, samples were left for 8 h at room temperature (aging) and cured in oven at 60 °C for 6 h to ensure complete curing. In the next step, in order to confirm the anticorrosive efficiency of the organic inorganic hybrid coating, potentiodynamic polarization curves were obtained after 30 hours immersion in 3.5% NaCl solution.

The bare 304 stainless steel presented a current density of  $2.16 \times 10^{-7}$  A.cm<sup>-2</sup> and corrosion potential of -0.67 V, while the 1:0.8 Wt% HTEOS/Epoxy resin hybrid coating showed reduction of the current density to  $2.28 \times 10^{-8}$  A.cm<sup>-2</sup> and potential to -0.45 V. These results demonstrate an improved corrosion protection for hybrid coating compared to uncoated 304 stainless steel.

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## Electrodeposition Of G-C<sub>3</sub>N<sub>4</sub>/MoS<sub>2</sub> Nanocomposites For Application In Bulk Heterojunction Polymer Solar Cells

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Bulk heterojunction Polymer solar cells (BHJ PSCs) are considered promising energy power suppliers in recent years due to their light weight, printability, low-energy fabrication and high flexibility. BHJ PSCs consists of cathode / active layer / anode. Hole transporting layer (HTL) and electron transporting layer (ETL) are entered into the structure to improve the performance of the BHJ PSC. Here for the first time we demonstrate the use of g-C3N4/MoS2 nanocomposite as HTL in order to efficiently collect and transfer holes in BHJ PSCs. In the first step two precursors, melamine and urea, were used to prepare graphitic carbon nitride through a thermal decomposition (pyrolysis) method. G-C3N4/MoS2 nanocomposite were electrochemically grown on ITO using a potantiostatic method and then the effect of time of deposition were investigated. Finally, the synthesized samples were evaluated by XRD, SEM, AFM, CV and UV-Vis analysis.

The best devices were found to have an open circuit voltage (VOC) of about 0.54 V, short circuit current of 9.41 mA cm2, a fill factor of 64.3%, and a power conversion efficiency of 3.16%, which were, respectively, about 1.2%, 6.8%, 6.7% and 8.4%, compared to that considered for the reference device prepared base on the PEDOT:PSS HTL.



## Sunflower Petal Extract as an Anticorrosion Agent to Protect Carbon steel in The HCl Solution

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Metals corrosion is one of the major challenges in the different equipments at the oil, gas and petrochemical industries, that every year it is led to a lot of economic losses. Carbon steel is one of the most popular alloys used in the industrial equipment, because of it has mechanical strength and is economical. Usually for the pickling and de-scaling of alloys surface in the industrial devices , acidic solutions such as  $H_2SO_4$  and HCl have the most application [1].

Recently to reduce the effect of corrosion, the use of plants extract as a green and effective bioinhibitor is common, advantages of this plants extract are such as abundance in nature, renewability, nontoxic and low economical cost [2]. In current work, sunflower petal extract as a bioinhibitor to protect of carbon steel in HCl 1M solution is introduced. The inhibition performance was investigated by electrochemical experiments, include linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy. main components of sunflower petal extract were identified by gas chromatography coupled with a mass spectroscopy detector (GC-mass). The obtained results from polarization measurement showed that sunflower petal extract acts as an agent anticorrosion with an efficiency of 75% at the concentration of 5 % v/v inhibitor, and so corrosion resistance was examined by electrochemical impedance spectroscopy at the concentration of 5 % v/v.

Morphology of carbon steel surface in presence and absence of inhibitor was analyzed by scanning electron microscopy (SEM) the obtained observations showed that in presence of sunflower petal extract, on the surface of carbon steel less damage was occurred compared with

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HCl media, at the absence of inhibitor. The investigation of the adsorption isotherms showed that the Langmuir model is best matched for adsorption of sunflower petal extract over the surface of carbon steel ( $R^2 = 0.994$ ).

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### Electrochemical Hydrogen Generation by Silver-Palladium Coated Nickel Foam

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Population growth and urban development are led to declining global energy resources. On the other hand, fossil fuels, include oil, gas and coal which are main source of the world's energy, are finishing and so have high pollution. Among these, hydrogen can be mentioned as a suitable alternative to fossil fuels, one of the important advantages of hydrogen is burning without any pollution, because the product of burning hydrogen is water, so there is no pollution for the environment. Hydrogen electrochemical production was done from the water electrolysis by electrocatalyst[1].

One of the famous catalysts is platinum that is the best catalyst for hydrogen generation but it has disadvantages such as high economic cost and low abundance in the earth, for this reason researchers are developing electrocatalysts that can be replace platinum with other catalyst with good efficiency, stability, and low cost for hydrogen production[2].

In the current work, Pd And Ag as a bimetallic agent were deposited by electrochemistry method on polyaniline (PANI) as a conductive polymer coated over Ni foam and was used for hydrogen production in H<sub>2</sub>SO<sub>4</sub> solution with a concentration of 0.1 M. The morphology and chemical composition of the prepared electrodes were analyzed by field emission scanning electron microscopy equipped with energy-dispersive X-ray spectroscopy (FESEM-EDX). Electrochemical measurements include linear sweep voltammetry (LSV), electrochemical impedance spectroscopy (EIS), chronoamperometry (CA) and cyclic voltammetry (CV) were used for nickel foam modification and tested for hydrogen generation. The obtained results

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illustrated that AgPd bimetallic in the presence of PANI deposited on Ni foam has low  $\eta_{10}$  - 137 mV, the high current density of 162 mA.cm<sup>-2</sup> and high stability according to fast and easy electrode synthesis, the modification of electrode by AgPd is a suitable electrocatalyst in the hydrogen generation process.

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# Vanadium oxysulfide spheres on cobalt-cobalt sulfonitride nanosheets as efficient bifunctional electrocatalyst for oxygen and hydrogen evolution reaction

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Searching for alternative clean energy sources to address the scarcity of fossil fuels and environmental issues such as global warming and greenhouse gas emissions is an essential task for ensuring social health in the near future. So synthesis of efficient, low-cost, and stable bifunctional electrocatalysts with earth-abundant resources for electrochemical water electrolysis is a challenging subject for large-scale energy conversion processes. Herein, we report a high-performance electrocatalyst based on vanadium oxysulfide/cobalt-cobalt sulfonitride (VOS/Co-CoSN) for oxygen and hydrogen evolution reaction (OER and HER). The Co-CoSN film was synthesized on a copper sheet (CS) by a facile electrodeposition method. Then, VOS was electrochemically grown onto the Co-CoSN@CS electrode at various deposition times. At the optimal deposition time (300 s), the obtained VOS-300/Co-CoSN catalyst was studied for OER and HER in alkaline and acidic media, respectively. The binder free VOS-300/Co-CoSN@CS electrode showed significant improvement in catalytic activity towards both OER (Tafel slope of 0.201 V dec<sup>-1</sup> with overpotential of 0.34 V @100 A m<sup>-2</sup> current density in 1.0 M KOH media) and HER (Tafel slope of 0.048 V dec<sup>-1</sup> with overpotential of 0.18 V@100 A m<sup>-2</sup> current density in 0.5 M H<sub>2</sub>SO<sub>4</sub> solution). Additionally, the electrocatalyst exhibited high durability and flexibility for both OER (98 % stability after 24 h at 100 A m<sup>-2</sup>) and HER (99 % stability after 12 h at 0.18 V vs.RHE) in alkaline and acidic conditions, respectively. The present work not only suggests a simple and single-step strategy for the synthesis of VOS-300/Co-CoSN nanostructure but also opens up a new avenue for the development of bendable and stable bifunctional, non-noble metal electrocatalysts towards both OER and HER through water splitting procedure.



# Electrodeposition of nono-porous nickel selenide on graphite rod as a bifunctional electrocatalyst for overall water splitting

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The goal of this study is to use the cyclic voltammetry approach to construct the nano-porous structure of nickel selenide on a graphite rod substrate that is active for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). This is the first report of the production of this morphology as an efficient water splitting electrocatalyst on a graphite rod substrate using a quick, one-step, cost-effective electrodeposition process. First, by regulating the electrodeposition condition, a graphite rod was changed with nickel selenide nano porosity. The main outcomes reveal that the optimized Ni-Se coverage on graphite rod substrate illustrates hopeful HER activity with low overpotentials of -100.7, -281.3, and -552.9 mV at the current densities of -10, -100, and -400 mA. cm<sup>-2</sup>, respectively. Besides, the manufactured Ni-Se nano-porous catalyst is extremely active toward OER, needing overpotentials of only 268 mV for 10 mA. cm<sup>-2</sup> current density. This study presents a method for producing a novel nano-porous electrocatalyst as a highly active bifunctional water splitting electrocatalyst that is both cost-effective and quick. As a result of these findings, this electrocatalyst appears to be potential for creating green energy in an industrial setting.

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# Fabrication and Design of New Redox Active Azure A/3D Graphene Aerogel Electrodes for Supercapacitor

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Great efforts have been made to design and fabricate low-cost, high efficiency advanced electrode materials for energy storage devices such as batteries and high-performance supercapacitors. Choosing organic and redox active species that increase the Faradaic charge storage of electrode systems has thus become a challenge to increase energy density and conductivity. To this aim, herein, azure A/3D graphene aerogel (Az–GA) redox active electrodes are fabricated via a hydrothermal method .Az links to 3D GA via  $\pi$ – $\pi$  interactions to form an anode. The new electrodes were synthesized via a one-step hydrothermal process and electrochemically characterized via cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS) measurements. The Az–GA electrode exhibits good electrochemical performance and high specific capacitance of 716.06 F g<sup>-1</sup> at a current density of 1 A g<sup>-1</sup>.

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CVs of the Az–GA/NF electrode at various scan rates from 5 to 100 mV s<sup>-1</sup>, (inset: CVs of scan rates from 1 to 4 mV s<sup>-1</sup>) in a three-electrode cell setup in aqueous 3 M KOH electrolyte



GCDs of the (a) Az–GA/NF electrode at different current densities from 1–20 A g<sup>-1</sup> in aqueous 3 M KOH electrolyte, (b) Nyquist plots of the Az–GA/NF electrodes.

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# Fabrication and Design of New Conductive Trypan Blue–Nickel MOF Nanosheet Array Electrodes for rechargeable battery

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The use of renewable energy, such as solar and wind power, is of great importance to meet the energy demands of a growing population, as non-renewable energy sources dwindle and the general public gain more knowledge on environmental pollution. Electrical energy storage technology involves the storage of various forms of energy, including energy storage in electrochemical double-layer capacitors (EDLCs) and batteries. Batteries, including lithiumion batteries (LIBs), which were the topic of the Nobel Prize in Chemistry in 2019, present a great breakthrough in science and energy storage technology, and are essential for use in electronics and other technologies. Metal-Organic Frameworks (MOFs) have a high surface area of more than 7000 m<sup>2</sup> that of activated carbon, potentially allowing them to challenge the dominance of carbon activated electrodes in EDLCs. Due to the promotion of charge transfer within the structure of the MOF and the regeneration behavior of the metal cations, these nanostructures have been successfully used as electrode materials in energy storage devices. In this study, a Trypan (Try) blue-nickel MOF (Try-Ni-MOF) nanosheet array as a cathode. The new electrodes were synthesized via a one-step hydrothermal process and electrochemically characterized via cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS) measurements. In terms of the Try-Ni-MOF electrode, it exhibits a high specific capacitance of 845.43 F  $g^{-1}$  at a current density of 1 A  $g^{-1}$ . I 4<sup>th</sup> Biennial Electrochemistry Seminar of IRAN <sub>August</sub> 2021





CVs of the Try–Ni-MOF/NF electrode at various scan rates from 5 to 100 mV s<sup>-1</sup>, (inset: CVs of scan rates from 1 to  $4 \text{ mV s}^{-1}$ ) in a three-electrode cell setup in aqueous 3 M KOH electrolyte.



GCDs of the (a) Try–Ni-MOF/NF electrode at different current densities from 1–20 A g<sup>-1</sup> in aqueous 3 M KOH electrolyteand (b) Nyquist plots of the Try–Ni-MOF/NF electrode, in which the insets show magnified images of the high frequency regions.

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# Electrochemical deposition of V<sub>2</sub>O<sub>5</sub> nanorods for application in polymer based solar cells Fateme Hasannezhad, Leila Naji, Majid Arvand

Solar energy, with features like interminable and cleanness is the most promising technology to solve the energy crisis and achieve acceptable development. Among solar cells, organicbased solar cells are considered the next generation of technology to replace silicon-based solar cells. Among organic solar cells, bulk heterojunction polymer solar cells (BHJ PSCs) have become very popular. Many efforts have been devoted to developing BHJ PSCs due to their great low specific weight, ease of fabrication on a large area, compatibility with flexible substrates, low-cost, and low environmental hazardous. BHJ PSCs consist of three main substrates: photoanode, photoactive layer and cathode. The other two components which improve the PSCs' performance and stability are the electron transport layer (ETL) and the hole transport layer (HTL). The HTL task is to improve the anode's efficiency in collecting and extracting the holes in BHJ PSCs. The HTL selectively transmits the positive charge, and so it prevents the passage of electrons towards the anode. The HTL should have good stability, high electrical conductivity, low resistance, and high working function. For current BHJ PSCs with indium tin oxide (ITO) as the anode, polyethylenedioxy thiophene: polystyrenesulfonate (PEDOT: PSS) has been widely used as the HTL due to its high work function and smoothing out the rough ITO film. Unfortunately, the strong acidity of PEDOT: PSS causes problems such as heterogeneous corrosion of electrical structures and degradation of cell stability. Recently, the use of transition metal oxides (TMOs) as a replacement of (PEDOT: PSS) in the hole transport layer (HTL) of bulk heterojunction polymer-based solar cells (BHJ PSCs) have received much attention. The current work describes a low cost solution-based electrochemical deposition method to synthesize vanadium pentoxide (V<sub>2</sub>O<sub>5</sub>) nanorods (NRDs) and their application as HTL in BHJ PSCs. V<sub>2</sub>O<sub>5</sub> nanostructures were electrochemically grown on the ITO electrode using cyclic voltammetry method and the structural, morphological, optical, and electrochemical properties of the synthesized  $V_2O_5$  nanostructures were compared. The charge transfer and charge recombination rate of the active layer-coated samples were investigated using electrochemical impedance spectroscopy and photoluminescence spectroscopy techniques. V<sub>2</sub>O<sub>5</sub> NRDs formed a three-dimensional microporous network with orthorhombic structure on the ITO and showed electroactive surface area of 0.22 cm<sup>2</sup>, excellent conductivity of 0.04 mS. cm<sup>-1</sup> and charge mobility of 2.27×10<sup>-3</sup> cm<sup>2</sup>.V<sup>-1</sup>s<sup>-1</sup>. The best V<sub>2</sub>O<sub>5</sub> NRDs-based device showed a short circuit current of 9.21 mA cm<sup>2</sup>, a open-circuit voltage of 0.54 V, a fill factor of 63.5%, and a power conversion efficiency of 3.18%, which were, respectively, about 2.2%, 6.9%, 5.2% and 3%, compared to that considered for the reference device prepared base on the PEDOT: PSS HTL.



# Preventing Corrosion In Pipes By Treating Water In Crude Oil Emulsion Using Silica Modified By Cationic Surfactant

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The crude oil extracted from reservoirs is usually accompanied by the water droplets in the form of stable water in oil (w/o) emulsion. The stability is due to existence of natural surface active materials (asphaltene and resin) in crude oil. This harmful emulsion is the cause of catalyst poisoning and corrosion in pipes and pumps, therefore the water droplets should be removed before entering to petrochemical industries. Chemical demulsification is one of the best methods to treat water in oil emulsion, since it is cost-effective, efficient and facile [1].

In this work, silica is modified using surface active agent to remove stable water in crude oil emulsion. The emulsion contained 70% crude oil and was at least few months stable.

FTIR results showed the right synthesis of the cationic surfactant on Silica. Interfacial tension between water and crude oil was decreased significantly after adding demulsifier, showing that the demulsifier is highly active in interface. Bottle test showed that silica modified by surfactant can separate 100% water from crude oil in 50 minutes, 33% faster that silica alone. The cationic surfactant of the demulsifier attach to the water droplets surrounded by negative oil droplets, causing droplets coalescence. This demulsifier is cost-effective, environment friendly and highly efficient in treatment of water in crude oil emulsion, showing great potential to be used in industries.

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# Investigation the Effect of expander content on the cycle life of lead acid battery

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In recent decades, more and more electronic systems (start-stop, drive-by-wire, brake-bywire) have been developed in the automotive industry therefore reliable power sources are necessary. It is essential to understand thoroughly the detailed behavior of the battery to increase its efficiency and cycle life. With modern battery design it is not enough to improve the positive active material performance only, it is quite clear that the negative active matrial also has to meet new requirements. Negative plate of lead acid batteries are produced by applying a paste of leady oxide, expander, water, and diluted sulphuric acid onto a lead or leadalloy grid structure. By use of formation process, cured past convert to electrochemically active porous material i.e. sponge lead as negative plate. In this investigation negative paste preparation is carried out with different content of expander. Negative active material was characterized by capacity, cycle life, cold cranking ampere and SEM analyses. Result shows that by increasing of barium sulfate and decreasing of lignosulfonate content of expander, Capacity and cold cranking of negative active material decreased but cycle life increased.

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# SiO<sub>2</sub>/N-doped graphene composite derived from metal organic framework as anode in lithium-ion batteries

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Silica  $(SiO_2)$  is a very promising anode material for lithium-ion batteries, due to the advantages of resource-rich, high theoretical specific capacity and suitable reaction voltage. However, its large volume expansion effect severely limits its commercial application. Therefore, surface modification and smart structural designs, such as nanostructures, core-shell structures and silica -carbon composite structures, are some of the most effective ways to solve the serious volume expansion effect of silica anode materials. In recent years, metal oxide anode materials derived from organic frameworks have been extensively studied. They have porous structures and abundant carbon materials, which can effectively enhance conductivity and alleviate the volume expansion. In this work, Nano SiO<sub>2</sub>@ Zeolitic imidizolate framework-67 (ZIF-67)-700@SiO<sub>2</sub>-700 double composites were successfully prepared by a facile co-precipitation, thermal treatment process and Stöber method. When this double composites had been two stages of pyrolysis at 700 °C and been used as an anode material in a lithium-ion battery, it delivers a high specific capacity of 510 mAhg<sup>-1</sup> after 250 cycles at 0.5 Ag<sup>-1</sup> and show excellent electrochemical performances in terms of high reversible capacity, superior cycling stability, and good rate capability. The surface modification results of this work provide a new way to solve the volume expansion effect of a Silica anode material. In addition, the corresponding electrochemical reaction mechanism is investigating as shown in in Fig.1. This approach provides a means of improving the electrochemical performance of lithium-ion battery.





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Fig.1: a) Galvanostatic charge–discharge voltage profiles of the Nano SiO<sub>2</sub>@ZIF-67-700@SiO<sub>2</sub>-700 electrode at a current density of 0.5 Ag<sup>-1</sup> for 1<sup>st</sup> cycle. b) Cyclic voltammetry (CV) curves for Nano SiO<sub>2</sub>@ZIF-67-700@SiO<sub>2</sub>-700 electrode scanned at the rate of 0.1 mV s–1.

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# Novel electrocatalysts for borohydride fuel cells: enhanced power generation by optimizing Bimetallic Ni-Co nanoparticles on Nickel Foam (NF)/ reduced graphene oxide

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The generated power density in direct sodium borohydride–hydrogen peroxide fuel cells (DBFCs) using non-precious metals such as Co or Ni as the anodic catalyst is low. Among the non-precious metals, Ni has attracted much attention because of its high activity for borohydride adsorption, high persistence under alkaline conditions, and negative potentials. In this research, the effects of graphene reduced oxide, electrocatalyst's performance and the performance of (DBFCs) are studied in detail.

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Bimetallic Ni-Co nanoparticles on Nickel Foam (NF) reduced graphene oxide are fabricated by electrodeposition to be used as anode electrocatalysts for (DBHPFCs). The physical characterization of synthesized materials is investigated using Fourier transform infrared spectroscopy, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and X-ray diffraction. The electrochemical half-cell tests are used to study their electrocatalytic properties toward borohydride oxidation in an alkaline solution. Finally, a direct sodium borohydride– hydrogen peroxide fuel cell is assembled using Pt/C as a cathode and Ni-Co/ rGO as an anode. Maximum power density values of 308 mW cm<sup>-2</sup> at 60 °C are obtained for Ni<sub>50</sub>-Co<sub>50</sub> /rGO. Thus, this study revealed that Ni<sub>50</sub>-Co<sub>50</sub> /rGO is a suitable anodic electrocatalyst for application in DBHPFCs in comparison with the commercially used Pt-based electrocatalysts because of its advantages such as low cost, high activity toward the BOR and stability in fuel cells.

**Keywords**: Ni–Co nanoparticles ,direct borohydride–hydrogen peroxide fuel cell, borohydride oxidation reaction, Nickel Foam.

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# $\label{eq:expectation} Evaluation the \ conductivity \ behavior \ of E7 \ nematic \ liquid \ crystal \ doped \\ with \ MgMn_2O_4 \ nanoparticles$

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Abstract: Dispersing nanoparticles (NPs) into liquid crystals (LCs) is increasingly studied as method to enhance the physical and electro-optical properties of LCs and produce new functional materials with widespread applications in photonics and biotechnology.[1-3] Typical examples of doping NPs, incude ferroelectric NPs, metallic NPs inorganic NPs, and in particular ferronematics, i.e. stable cololoidal suspensions of fine magnetic particles in nematic liquid crystals (NLCs) which were first theoretically pointed out by Brochard and de Genns [4] that the colloidal particles prossess a permanent magnetic moment with the orientation of the local moment would be coupled with the NLCs direction. In the present study, the conductivity and Resistance of pure liquid crystal E7 and its mixtures with different percentage (0.5, 1 and 1.5 W/W%) of MgMn<sub>2</sub>O<sub>4</sub> nanoparticles were investigated. The impedance of each of the pure and doped liquid crystal samples were measured. Analysis of the obtained data showed that by increasing the concentration of MgMn<sub>2</sub>O<sub>4</sub> to 0.5wt. the conductivity was increased significantly. while, in higher 0.5 wt.% concentration of MgMn<sub>2</sub>O<sub>4</sub> the conductivity was decreased. However, in all doped samples, the value of conductivity are higher was compared to pure E7 nematic liquid crystal. In other word, the E7@MgMn<sub>2</sub>O<sub>4</sub> showed promising electrical conductivity was compare to pristine E7 nematic liquid crystal due to absorption of ionic impurities by MgMn<sub>2</sub>O<sub>4</sub>.



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Figure 1: Nyquist curves of LCs containing various weight percentages of  $MgMn_2O_4$ . Symbols

illustrate the measured data. Solid curves demonstrate the fitted results obtained from the simulations based on the equivalent circuit model shown in the inset

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# Electrochemical characterization of binuclear ruthenium (II) complex towards application in light-emitting electrochemical cells (LECs)

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Light-emitting electrochemical cells (LECs) are thin-film lighting devices that consist of an active layer sandwiched between two air-stable electrodes. These devices have recently attracted significant attention due to their great potential for use in illuminations and displays technology [1]. The active layer in LEC devices can be conjugated polymers, ionic transition metal complexes (iTMCs), quantum dots, etc. Among these emitter materials, iTMCs possess several superior properties such as stable redox properties, intrinsically ionic feature, phosphorescent nature of iTMCs that results in more efficient electroluminescence (EL) [2]. Therefore, a significant number of attempts have been made in the improving electroluminescence features of LECs via the modification of the molecular structure of iTMCs. Although LECs have many advantages, however, they suffer from some limitations such as low stability. To overcome this limitation, the increasing of the number of metal core to produce multi nuclear ruthenium complexes is a promising way to increase the stability of LEC device [3].

In this work, we designed and synthesized a new binuclear ruthenium complex with bipyridine as an ancillary ligand. To investigate the redox properties of this binuclear complex as well as the finding of an insight into the electronic structure, cyclic voltammogram of the complex was I 4<sup>th</sup> Biennial Electrochemistry Seminar of IRAN <sub>August</sub> 2021



recorded in acetonitrile solution and nNBu<sub>4</sub>ClO<sub>4</sub> as the supporting electrolyte. The electrochemical data are given in Table 1. As shown in the cyclic voltammogram, the binuclear complex depicted a unique reversible oxidation peak in the anodic potential region which is ascribed to the oxidation of the Ru(II) to Ru(III). In the cathodic region, several reversible and irreversible reduction peaks at -0.7 V to -1.6 V were observed, which can be assigned to the one-electron reduction processes localized on polypyridyl ligands [4]. The reversible redox processes in positive and negative potential predict high stability of this complex under the operation conditions used in LEC device owing to the reversible nature of the red/ox process in which the complex is involved in those devices [5, 6]. The linear correlation between the square root of scan rate ( $v_{2}$ ) and the anodic current shows that the kinetics of the overall process is controlled by mass-transport phenomena in solution. In the following, we estimated the energy of frontier orbital levels (Highest occupied molecular orbital (HOMO) and lowest unoccupied orbital molecular (LUMO),) and band gaps of the complex by use of the electrochemical and photophysical data (see Table 1) [7].

Tabl	Table 1. Electrochemical features of emitter.					
Com	Ru (II/III) Oxidation.		E0-0 <sup>c</sup>	Еномо <sup>d</sup>	ELUMO <sup>e</sup>	$\mathbf{E_{gap}}^{\mathbf{f}}$
Com.	$E_{1/2} (V)^a$	$\Delta E (V)^{b}$	(eV)	(eV)	(eV)	(eV)
Binuclear Ru(II)	1.33	0.070 <sup>g</sup>	2.31	-5.74	-3.43	2.31

<sup>a</sup> From CV measurements,  $E_{1/2} = \frac{1}{2} (E_{pa}+E_{pc})$ ; 0.1 M acetonitrile/TBAP versus Ag/AgCl. <sup>b</sup>  $\Delta E = E_{pa}-E_{pc}$ . <sup>c</sup> From the intersection of absorption and emission spectra. <sup>d</sup> From the formula  $E_{HOMO} = [-e(E_{ox} - E_{1/2} (Fc/Fc^+)] - 4.8 eV$ . <sup>e</sup> From the formula  $E_{LUMO}=E_{HOMO}+E_{0-0}$ . <sup>f</sup> $E_{gap}=E_{HOMO}$ -  $E_{LUMO}$ . <sup>g</sup> An reversible electtrochemical process.

LEC devices were fabricated by spin coating the complex and a suitable hole injection layer on an ITO with the structure of ITO/PEDOT: PSS/complex/Ag. The LEC device showed a deep red emission centered at  $\approx 680$  nm and the turn-on voltage of 2.5 V. The electroluminescence data of LEC based on the binuclear complex as emitter, are summarized in table 2. The binuclear Ru(II) Complex yielded electroluminescent devices of appreciable brightness and stability compared with similar complexes [3].

Table 2. Electroluminescent characteristics of the ELC Device.							
Device.	$\lambda_{max, EL} (nm)$	CIE [x, y] <sup>a</sup>	$V_{on}{}^{b}$	$t_{1/2}^{c}$	t <sub>on</sub> <sup>d</sup>	J e	
1	680	[0.734, 0.265]	2.5	15	120	264	
<sup>a</sup> Commission Internationale de l'Eclairage color coordinates, 1931. <sup>b</sup> Turn-on voltage (onset voltage							
obtained at 10 <sup>-4</sup> mW.cm <sup>-2</sup> ) (V). <sup>c</sup> Lifetime (minute) at 5 V. <sup>d</sup> Turn-on time to reach maximum radiance at 5 V							
(second). <sup>e</sup> Current density (mA $cm^{-2}$ ) at 5 V.							

Table 2. Electroluminescent characteristics of the LEC Device.

Conclusion:

In this study, we reported the new binuclear ruthenium (II) complex and we investigated its electrochemical properties. Electrochemical data showed the reversible red/ox behavior of complex and thus the good stability of the two species (Ru(II, II)) as one of the most important

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features of iTMC in light-emitting electrochemical cells. This complex was used as an emitter in the LEC device and showed stable and high brightness red emission. The results showed that the positive effect of uncoordinated pyridine moiety and increasing the metal core on electroluminescence features of iTMC in LEC.

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# Facile synthesis of NiMgMn<sub>2</sub>O<sub>4</sub> composite as a high-Performance electrode for Mg-ion battery.

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Aqueous magnesium ion batteries feature good safety and high energy density and represent a promising kind of energy storage system<sup>[4]</sup>. The need for safe, cost-effective aqueous magnesium ion batteries has led to high electrochemical performance designs of materials and structures to meet strict requirements. However, optimized electrodes are the key to realize its advantages. In this work, we report a Ni-doped Magnesium manganese oxide (MgMn<sub>2</sub>O<sub>4</sub>) as the cathode via a self-template method, which help to improve conductivity and solve defects derived from pristine MgMn<sub>2</sub>O<sub>4</sub> with nickel doping<sup>[1]</sup>. This electrode exhibits excellent electrochemical performance in a MgSO<sub>4</sub> electrolyte. Moreover, this cathode can obtain an initial discharge capacity of 164.15 mAhg<sup>-1</sup> at a current density of 500 mAg<sup>-1</sup> and a cycling stability with 57.63% capacity retention after 250 cycles. Therefore, the assembly of an aqueous magnesium ion battery with excellent rate performance is based on three electrodes. In addition, the corresponding electrochemical reaction mechanism is investigating as shown in in **Fig.1b**. This approach provides a means of improving the electrochemical performance of Mg battery systems.



**Figure 1**: a) cyclic performance for two sample  $MgMn_2O_4(red)$  and  $MgMn_2O_4@Ni_{0.25}(green)$  in current density 500 mAg<sup>-1</sup> for 250<sup>th</sup> cycle. b) CV curve for two sample  $MgMn_2O_4(red)$  and

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 $MgMn_2O_4@Ni_{0.25}$ (green) with rate 0.5 mV from potential -0.6 to 1.2 V Vs. reference electrode Ag/AgCl.

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# Fabrication of stable and low-cost HTM-free full mesoscopic CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> perovskite solar cell containing ZrO<sub>2</sub> as spacer layer

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In the past few years, organic-inorganic perovskite solar cells (PSCs) have been improved drastically in terms of solar to electric power conversion efficiency (PCE) and stability. Mesoscopic carbon-based perovskite solar cells (C–PSCs) have emerged as the most promising candidates for commercialization in the field of perovskite photovoltaics, as they are highly stable, low cost, and make use of easily scaled manufacturing techniques. In this research, effect of the ZrO<sub>2</sub> spacer layer on the photovoltaic performance of mesoscopic CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> perovskite solar cells was investigated. The architecture of prepared cell was mp-TiO<sub>2</sub>/mp-ZrO<sub>2</sub>/mp-Carbon architecture. We avoided using hole-transporting materials (HTMs) and Au as a counter electrode. In this case, ZrO<sub>2</sub> acts as a spacer layer between TiO<sub>2</sub> and carbon layers. As a result, full mesoscopic perovskite solar cell has a high current density and voltage compared to the cell without ZrO<sub>2</sub> layer. The photoelectric conversion efficiency of 5.33% was obtained with the hole-conductor-free fully mesoscopic perovskite solar cell.

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Fabrication method: FTO glass was used as an anode. Initially, the thin layer of titanium oxide as a blocking layer is deposited on the FTO substrate using the spin-coating method (2000 rpm, 20 s) and annealed at 450 °C for 30 min. Then, the mesoporous TiO<sub>2</sub> layer was prepared with diluted TiO<sub>2</sub> paste (w/w=1:3.5 in ethanol) by spin coating on the blocking layer at 5000rpm for 30s and heated at 500°C for 60min. The mesoporous  $ZrO_2$  layer was prepared with diluted  $ZrO_2$  paste (w/w=1:5 in ethanol) by spin coating on the mesoporous titanium oxide layer at 2000rpm for 30s and heated at 500°C for 60min. In the next step, the mesoporous carbon layer was prepared with carbon paste by doctor-blading on the zirconium oxide layer and heated at 400°C. Finally, 10µL of the perovskite solution was dropped on the top of the carbon electrode, where it infiltrated through the pores, and at the end, it was annealed at 70°C for 1 hour. The I-V curve was recorded in -1 to 1 V under illumination of solar light by the solar simulator (AM1.5G).

EIS Nyquist plot demonstrated that the charge transfer resistance in full mesoscopic type was lower and recombination resistance was higher than the cell without  $ZrO_2$  layer. Photovoltaic parameters such as the open-circuit voltage (V<sub>oc</sub>), short-circuit photocurrent density (J<sub>sc</sub>), fill factor (FF), and power conversion efficiency (PCE) were obtained. The open-circuit voltage (V<sub>oc</sub>) of full mesoscopic type was obtained 700 mV.

Cell	I <sub>sc</sub> (mA/cm <sup>2</sup> )	Voc (V)	FF (fill factor)	Efficiency (%)
mpTiO <sub>2</sub> +MAPbI <sub>3</sub> /mpZrO <sub>2</sub> +MAPbI <sub>3</sub> /mpCarbon+MAPbI <sub>3</sub>	13.79	0.7	0.55	5.33
mpTiO <sub>2</sub> +MAPbI <sub>3</sub> /Carbon	4.1	0.65	0.53	1.42

In summary, we have designed and implemented a facile method to deposit high-quality mesoporous TiO<sub>2</sub>, ZrO<sub>2</sub>, and Carbon layers via delayed annealing treatment and infiltrating perovskite material through the pores of mesoporous layers. Moreover, by taking advantage of the mp-ZrO<sub>2</sub> that acts as a spacer layer between mp-TiO<sub>2</sub> and mp-carbon layer to prevent short circuit and its advantage to provide more area for harvesting light by perovskite, we fabricate more stable and cheaper mesoscopic PSCs with appropriate absorption of the perovskite absorber.

Keywords: Perovskite, Full-Mesoporous, HTM-free, Carbon-based solar cell, PSCs

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# Electrooxidation of Ethanol on non-precious electrocatalyst 3D CoCu-MOF material

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The world has begun to gain out alternatives for renewable energy sources to certify consistent economic improvement by reduction of fossil fuel. A fuel cell system powered by some cheap fuel such as ethanol is one of the environmentally friendly ideal energy systems for reasons of their high thermodynamic efficiency, easy storage, low cost, and toxicity. Accordingly, the development of useful and stable electrocatalysts for the anodic ethanol oxidation reaction (EOR) is important. The expansion of bifunctional metal-organic frameworks (MOFs) with transition metal for the ethanol oxidation reaction (EOR) is highly favorable because furnish an opportunity for the construction of mixed metals dispensation in the carbon frame without any carbon precursor augmentative. Herein, we present a three-dimensional (3D) flower-like CoCu MOF, and the prepared sample was used as a non-precious electrocatalyst for Ethanol oxidation reaction. The morphologies of all samples were investigated by a scanning electron microscope (SEM) and energy-dispersive X-ray (EDX) spectroscope. X-ray diffraction (XRD) data for measuring the crystallographic structures and phase purity. The composition of asprepared samples was revealed by Fourier transformation infrared spectra (FTIR). Electrochemical experiments were carried out in a three-electrode system with an Origa Flex-OGF 01A Potentiostate/Galvanostate set up. A certain amount of catalyst powder was

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dispersed in ethanol and Nafion (5 wt.%) to form a homogeneous ink. Then, certain amount of ink dropped onto the commercially available glassy carbon electrode (GCE, d=0.126 mm) and used as a working electrode. For each catalyst EOR measurements were recorded in 1 M NaOH solution containing 0.5 M EtOH. The EOR activity of catalysts is investigated via cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), chronopotentiometry, and chronoamperometry techniques. The resulting show that, CoCu in comparison to the monometallic Cu and Co MOFs arrives at the remarkable area-specific activities of 2.589 mA cm<sup>-2</sup> at scan rate 20 mV.s<sup>-1</sup> toward the anodic oxidation of ethanol. EIS test statements that the CoCu-MOF has the lower impedance. Chronoamperometry express CoCu-MOF has better stability comparative to Cu and Co MOF. The individual 3D flower-like structure of MOF with free pores, high specific surface area, and synergistic effect between Co and Cu contribute to the highest EOR activities of the present work. This catalyst is a good candidate for use in liquid fuel cells with ethanol fuel.

Keywords: CoCu MOF, Metal-Organic Frameworks, Ethanol, Electrocatalytic oxidation.

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# Organic acid doped polypyrrole - natural Ilmenite (FeTiO<sub>3</sub>) nanocomposite on Titanium substrate as an efficient photoanode for solar photoelectrochemical water splitting

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In recent years, the solar induced photoelectrochemical (PEC) water splitting has been attracted a lot of attention due to its great capability in direct conversion of clean and renewable solar energy into chemical energy (hydrogen and oxygen generation) by the use of appropriate semiconductor materials. Construction of conductive polymer-inorganic metal oxide heterojunctions with matching energy levels enabling fast charge separation and transfer is a good strategy that benefits from the properties of both organic and inorganic semiconductors. In this research, the nanocomposites of camphor sulfonic acid doped polypyrrole (CSA PPy) as organic semiconductors with natural Ilmenite (FeTiO<sub>3</sub>) as inorganic semiconductor were synthesized using in-situ oxidative polymerization. The morphology and structural properties of as-synthesized nanocomposites were investigated by Fourier transform infrared (FTIR) spectroscopy, Raman spectroscopy, X-ray diffraction (XRD), and Field emission scanning electron microscopy (FESEM). The photoelectrocatalytic performance of Ti/CSA PPy, Ti/FeTiO<sub>3</sub>, and Ti/CSA PPy-FeTiO<sub>3</sub> were evaluated as photoanode by linear sweep voltammetry (LSV), chronoamperometry (CA), and electrochemical impedance spectroscopy (EIS) toward photoelectrochemical water splitting in dark and light under Xenon lamp (power I 4<sup>th</sup> Biennial Electrochemistry Seminar of IRAN <sub>August</sub> 2021



density:100 mW/cm<sup>2</sup>) conditions. All the electrochemical tests were carried out using threeelectrode set up by Origa flex 01A Galvanostat - Potentiostat in NaOH 1 M.

The Ti/CSA PPy-FeTiO<sub>3</sub> electrode shows the considerable photoelectrochemical response toward oxygen evolution reaction (13.78 mA/cm<sup>2</sup>) which is 1.21, 4.01 times higher than that of Ti/CSA PPy (11.35 mA/cm<sup>2</sup>) and Ti/FeTiO<sub>3</sub> (3.44 mA/cm<sup>2</sup>), respectively. Also, the onset potential of water oxidation on the Ti/CSA PPy-FeTiO<sub>3</sub> shifts towards lower values in comparison with two other electrodes. The formation of type II heterojunction between FeTiO<sub>3</sub> and CSA PPy allows the separation of charge carriers easier and faster. The EIS results indicated that charge transfer resistance (R<sub>ct</sub>) values Ti/CSA PPy, Ti/FeTiO<sub>3</sub>, and Ti/CSA PPy-FeTiO<sub>3</sub> at electrode/electrolyte interface under illumination are 79.49  $\Omega$ cm<sup>2</sup>, 227.7  $\Omega$ cm<sup>2</sup>, and 58.69  $\Omega$ cm<sup>2</sup>, respectively. The combination of FeTiO<sub>3</sub> and CSA PPy decreased the charge transfer resistance compared to pure FeTiO<sub>3</sub> and CSA PPy which has the synergistic effect on the interfacial separation of electron and holes in the electrode/electrolyte interface. As a result, Ti/CSA PPy-FeTiO<sub>3</sub> can be considered as efficient organic-inorganic semiconductor for photoelectrochemical water splitting.

Keywords: Polypyrrole, Natural FeTiO<sub>3</sub>, Water Splitting, Photoanode, Titanium.

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# Improving the power conversion efficiency of Nonfullerene bulk heterojunction solar cell containing polyaniline-WO<sub>3</sub> nanocomposite as active layer by embedding reduced graphene oxide

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The development of hybrid polymer semiconductor compounds as active substances in solar cells is one of the most important fields of renewable energy researches. In this regard, the synthesis of new polymer nanocomposites with diverse morphology and high performance in order to improve the efficiency of hybrid polymer solar cells has attracted the attention of many researchers. In this study, camphor sulfonic acid doped polyaniline - tungsten oxide (CSA PANI-W) nanocomposite was synthesized by in situ oxidative polymerization. Then, the reduced graphene oxide was embedded into CSA PANI-W nanocomposite (CSA PANI-W-rGO) by electrochemically reduction of GO to rGO under light irradiation. Actually, the semiconductive nature of CSA PANI-WO<sub>3</sub> was used for photo reduction of GO to rGO. The Fourier transform infrared (FTIR) spectroscopy, Raman spectroscopy, X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), transmission electron

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microscopy (TEM) and X-ray photoelectron spectroscopy (XPS) techniques were used for characterization.

The synthesized compounds were used as the active layer in hybrid polymer solar cells with the structure of Indium-doped tin oxide (ITO) as the photoanode/polyethylene dioxythiophene: polystyrene sulfonate (PEDOT: PSS)) as a hole transfer layer/active layer (CSA PANI-W) and (CSA PANI-W-rGO)/Ag as cathode. The layers of cells were coated using spin coating technique. The final Ag layer was deposited by physical vapor deposition (PVD) method. The photovoltaic properties of prepared solar cells were evaluated using current-voltage (J-V) curves and obtaining relevant parameters such as open circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE). Electrochemical impedance spectroscopy (EIS) analysis was performed in 100 mHz - 100 kHz with Origa flex 01A (Origa, France) instrument to further investigate the charge transfer process in interfaces as well as the lifetime of charge carriers in prepared polymer hybrid solar cells. All of the tests were performed under simulated sunlight which was provided by Sharif Solar Simulator with AM 1.5G filter and 100 mW/cm<sup>2</sup> power density. The PCE of solar cells containing CSA PANI-W and CSA PANI-W-rGO were 0.848 % and 1.574 % indicating the enhancement of the photovoltaic performance in the presence of rGO.

The charge transfer resistance for the cell containing CSA PANI-W is  $0.36 \text{ k}\Omega \text{cm}^2$ , which is 1.38 times larger than a cell with an active layer containing CSA PANI-W-rGO ( $0.26 \text{ k}\Omega \text{cm}^2$ ) nanocomposite. It can be concluded that the presence of rGO causes effective transferring and separation of charge carriers, improvement of photovoltaic parameters and cell efficiency. Therefore, reduced graphene oxide is a good option to replace fullerene and make low-cost hybrid polymer solar cells.

Keywords: Polyaniline, Reduced graphene oxide, WO<sub>3</sub>, BHJ, Solar cell.

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# Carbon Shell Derived from Poly Acrylic Acid in Comparison with Poly Dopamine On prickly-Nickel Nanowire: Fabrication, Characterization and Application for Hydrogen Evolution Reaction

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As the theme of the day, hydrogen evolution reaction (HER) has been considered as a prototype reaction regarding electrochemical kinetic and catalytic performance researches and surveys. Moreover, HER is considered as a rational strategy for H<sub>2</sub> production for decreasing the total cost of hydrogen through reduction of the electrode reaction overpotential. Therefore, electrocatalysts based-on non-precious metals with high activity towards hydrogen evolution reaction (HER) are desirable approach toward renewable energy devices such as fuel cells and water electrolysis. Nevertheless, fabrication of state-of-the-art materials for such purposes remains a tremendous challenge. Here, two different binder-free composites based on prickly

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nickel nanostructure core decorated with carbon shell derived from poly acrylic acid and poly dopamine is constructed. The prickly nickel core structure were successfully synthesized through two different synthesis procedure. Next, both produced platforms were compared with each other regarding their electrocatalytic activity and were tested successfully for the HER in alkaline solution. Furthermore, structures as well as activities of the fabricated composites were characterized quantitatively by electrochemical methods and surface techniques. The attained FE-SEM images of the prickly nickel nanostructures confirms the successful production and their morphology. A wide variety of electrochemical technique such as cyclic voltammetry, linear sweep voltammetry and galvanic charge-discharge were also applied. In effect, the composites have shown excellent electrocatalytic activity toward the HER which were confirmed through Tafel slope, exchange current density (j<sub>0</sub>), and electrode reaction overpotential  $(\eta)$ . The superior increase in the electrocatalytic activity was found to be originated partially from increase in the surface roughness of the nanostructure and mainly from increase in the synergistic chemical coupling effects between prickly nickel nanostructures and carbonized shell that covered the whole structures. In another word, nickel nanowires and prickly nickel nanowires have been studied to escalate the effective surface area of the electrode and in turn promote the performance of the HER.

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# **Beware of Fourth Generation of Nickel Plating Brightener**

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The use of organic compounds as addition agents in aqueous electroplating baths is a fascinating field, mainly to interesting and important effects produced on the growth and structure and thereby on the character of the deposit by very low concentrations of the additives in the bath.

The striking effects on electrocrystallization processes of small concentrations of addition agents point to their adsorption on a high energy surface and deposition on growth sites, thereby producing a poisoning or inhibiting effect on the most active growing sites.

In this paper, the characteristic of the fourth generation of nickel brightener additive which produce bright nickel plate will be discussed with respect to their molecular structure.

In 1936, the commercial use was started from an aromatic sulfon-compound (p-toluene sulfonamide) together with an unsaturated aldehyde as the brightening system in a Watts nickel bath. The key to modern bright nickel plating was the discovery of the conjoint use of an organic sulfon-compounds with compounds with unsaturated functional groups that produced brightness and leveling in their conjunctive use.

Generally Nickel plating brightener was divided into four generations. First generation nickel plating brightener is take metal-salt as main additive; The second one that was combined of the 1.4-butynediol and Saccharin; The third generation was epoxy compounds and 1.4-butynediol with Saccharin; In the 4th generation, is take the combination of pyridine derivatives, alkynyl amines compounds and propargyl alcohol derivative.

After studying the influence of many organic additives, it was determined that some organic groups were more effective. In this respect, molecules that contain triple bonds are known to show good adsorption ability to metal surfaces via the  $\pi$  electron. Although all molecules have



triple bonds, functional groups such as alcohol (PA), ethoxylate (PME), sulfonate (PS) and dietylamino (DEP) seem to have the adsorption ability of triple bonds.

All of these organic additives have the tendency to shift the Ni reduction potential to the negative area due to the presence of triple bonds in their structure, which facilitate their adsorption on the surface compared with single and/or double bonds.

The HOMO/LUMO energies and dipole moments obtained from theoretical calculations explained the better adsorption behavior of the molecules such as propargyl alcohol derivative to the surface at low current density, which consequently led to a brighter surface even at lower concentrations.

It can be seen that the synthesize of two or more organic compounds into a new substance, so that it has better surface characteristics suitable for the electrocrystallization process, especially the electron supply in the low current region, are the characteristics of the new generation of brighteners.

A significant feature of the fourth generation of nickel brightener is the very little amount of additives in the bath, less than 10 mg/L that reduced the decomposition products rate that greatly extended the processing cycle, which greatly improved the production efficiency and reduced waste. Also, the fourth generation of nickel brightener has strong enough leveling and wide current density range that improve the coverage into difficult areas even at low current density.

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# Ni-Co nanocones structure electrodeposited on nickel foam for high performance supercapacitors Shiva Moraveji, Farzaneh Bahmani, Lida Fotouhi

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In view of increasing levels of greenhouse gasses and environmental pollutions, there is a wellestablished need for an alternative clean energy source with high capacity and cycling stability. Accordingly, supercapacitors have gained a lot of attention due to their high power output, fast charging-discharging and environment friendly nature. Herein, a direct simultaneous deposition of Ni-Co nanocones on nickel foam substrate was performed by facile one-step electrodeposition method without any template, which causes an excellent electrical conductivity and efficiency of electrode materials. The electrochemical performance of the electrosynthesized nanocones was analyzed by cyclic voltammetry, galvanostatic chargedischarge and electric impedance spectroscopy in in 3 mol L<sup>-1</sup> KOH as aqueous electrolyte. The Ni-Co nanocone electrode demonstrates high specific capacitance at current density range of 2 to 20 A g<sup>-1</sup> with rate capability of 70% and reasonable cyclic stability of 83% at scan rate of 70 mV s<sup>-1</sup> after 10000 cycles owing the low internal resistance, and high surface area of nanocones. Interestingly, an asymmetric supercapacitor was fabricated by using Ni-Co nanocones as the positive electrode and active carbon as the negative electrode operating at the voltage window of 0–1.6 V deliver a high energy density of \*\*\* Wh kg<sup>-1</sup> at a power density of \*\*\* kW kg<sup>-1</sup>. We expect that our results will shed light on the promising insights into the electrical properties of nanocones in the application of supercapacitores.

Keywords: Supercapacitor, Nanocone, Nickel. Cobalt, Electrodeposition



# Turnip (Brassica rapa var. rapa L.) Bark Extract as a Green Corrosion Bio-inhibitor for Carbon Steel in 1 M HCl solution

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Carbon steel is one of the most important and useful alloys due to its economical price and good mechanical behaviors and its applications are widespread and used in many industries such as packing, crude pipeline manufacturing, and construction and many industrial procedures of descaling, acid pickling, and acidizing. Turnip (Brassica rapa var. Rapa L.) bark extract (TBE) has been introduced as a new, cost-effective, eco-friendly, easy to use, and effective natural inhibitor for carbon steel corrosion in 1 M HCl solution. To prepare the TBE water extract, microwave-assisted extraction (MAE) has been used and ethanolic extract of the turnip bark was obtained for gas chromatography-mass spectroscopy (GC-MS) analysis to determine its main molecular composition. The effect of the TBE on the corrosion rate of the carbon steel has been investigated using electrochemical impedance spectroscopy and potentiodynamic polarization analysis in real-time. The SEM-EDS analysis has been utilized

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to estimate the carbon steel surface changes due to the dissolution of the C-steel in the presence and absence of TBE and surface elemental evaluations, respectively. To obtain the optimum concentration of TBE for C-steel corrosion inhibition, various concentrations (i.e., 2.5 to 20% v/v) of TBE have been used in 1.0 M HCl solution as the corrosive media, and results obtained using electrochemical showed the highest inhibition efficiency (IE) of almost 91%. The efficiency of TBE on the C-steel corrosion in 1 M HCl solution in several higher temperatures (i.e., 298-338 K) has been studied and the IE% was 31.7% using 10% v/v of the TBE in 338 K. The adsorption mechanism of TBE on the C-steel evaluated using physicochemical studies, was found to be physical and followed Langmuir isotherm.

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# The evaluation of Carpobrotus. edulis leaf Extract as Eco-friendly Bioinhibitor for Copper Corrosion in 0.5 M NaCl solution

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Copper is one of the most important metals in many industries such as the shipping industry, especially in marine engineering due to its incredible mechanical, thermal, and electrical properties, so the copper corrosion can cause serve economic and environmental damages and so many affords have been done to reduce its corrosion. Green corrosion inhibitors attract so much attention in recent years due to their cost-effective, eco-friendly, easy preparation, and effective results. Carpobrotus. Edulis has been introduced as a novel and renewable source to produce green bio-inhibitor for the corrosion of copper in 0.5 M NaCl solution. To evaluate the inhibition effect of C. edulis leaf extract (CELE) on the copper in the mentioned corrosive media, the proper amount of the plant leaves was collected, washed, chopped into small pieces, and then mechanically squeezed to obtain CELE. Finally, 5 different concentrations of CELE were directly added to the 0.5 M NaCl solution to evaluate the corrosion rate of copper by

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electrochemical analysis such as electrochemical impedance spectroscopy and potentiodynamic polarization tests. Electrochemical impedance spectroscopy results showed that adding and increasing the CELE concentration leads to the increment of charge transfer resistance onto the copper active area resulting in a major reduction in copper dissolution and improving inhibition efficiency (IE%). The polarization results represent corrosion current density of copper in 0.5 M NaCl solution and showing that the addition of CELE leads to a kinetical control of corrosion. The highest IE% achieved was 87.35% using 20 v/v% of CELE which is promising. The mechanism of the copper inhibition, in this case, can be explained by the physical adsorption of CELE molecules on the copper surface. The CELE molecules can form a thin protective layer on the active area of copper which prevents Cl<sup>-</sup> ion attacks resulting in copper dissolution reduction. By evaluating the temperature effect on the copper corrosion in the absence and presence of CELE, it can be concluded that temperature increment leads to a serve increment of copper corrosion without CELE rather than the presence of it. Also, the IE% of CELE decreases in the higher temperatures which is refer to the desorption of CELE molecules from the copper surface due to the temperature increment. To validate the influence of CELE in reducing and inhibiting the corrosion of copper in 0.5 M NaCl solution, SEM-EDS analysis was utilized. The surface changes and elemental analysis using SEM-EDS showing that black spots which are referred to as corrosion damages, were reduced when CELE was used. Finally, C. edulis leaf extract is a suitable, easy-to-use, cost-effective, green, and practical inhibitor for copper corrosion in 0.5 M NaCl solution.

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# Nanostructured Polyaniline/Vanadium oxide composite hydrogel for high performance flexible supercapacitor

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In recent years, the demand of high performance flexible and portable electronics with high power and energy densities has increased rapidly. Currently, the flexible devices have seized the interest of researchers in energy storage especially, supercapacitors and batteries. Working on the same line, polyaniline/vanadium oxide-graphene oxide nanocomposite hydrogel was prepared as a potential electrode material for flexible supercapacitor. This nanocomposite hydrogel exhibited a high specific capacitance of 982.8 Fg<sup>-1</sup> at a current density of 2.7 Ag<sup>-1</sup> in H<sub>2</sub>SO<sub>4</sub> electrolyte. The symmetrical supercapacitor has shown high rate capability as well as excellent cycling stability. The excellent electrochemical performance of the present nanocomposites hydrogel has been realized due to well-designed cross-linked hydrogel structure, high surface area and synergic effects among all the constituents. This outstanding performance holds a great potential for next generation flexible supercapacitors.

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## The Effect of Turnip Bark Extract as Green Corrosion Bio-Inhibitor for copper dissolution in 0.5 M NaCl solution

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Turnip bark has been introduced as a novel, inexpensive, and green source to prepare an ecofriendly corrosion inhibitor for copper dissolution in the 0.5 M NaCl solution. Considering the importance of copper in many basic industries (i.e., agriculture, shipbuilding, construction, and chemical industry) and also environmental protection, many affords have been done to find turnip bark extract (TBE) as a green, economical and eco-friendly inhibitor that can be used for copper corrosion reduction in NaCl solution, easily and with high inhibition efficiency (IE%). For this purpose, TBE has been prepared by peeling the turnip bark and then washing, oven drying, and grinding it into a really fine powder with a particle size of 350 µm. Water extract has been produced by microwave-assisted extraction (MAE) of 4 g of the fine powder using 100 mL of DI water as a solvent in 70 °C and finally filtered with Whatman filter paper. To evaluate the corrosion process of copper in 0.5 M NaCl solution and the effect of TBE on it, electrochemical analysis such as potentiodynamic polarization (PP) and electrochemical impedance spectroscopy (EIS) has been done using 5 different concentrations of TBE in NaCl I 4<sup>th</sup> Biennial Electrochemistry Seminar of IRAN August 2021



solution, utilized by Potentiostat/Galvanostat device. The potentiodynamic polarization tests present the copper corrosion kinetically and thermodynamically. The addition of TBE into the corrosive solution leads to the reduction of copper corrosion current density and improvement of corrosion inhibition with the maximum IE% of 90.7% achieved by using 20 v/v% of TBE concentration. The EIS analysis has been utilized to evaluate the effect of TBE on copper corrosion in 0.5 M NaCl solution by evaluating the electrochemical parameters resulted from the best-fitted circuit of copper corrosion in NaCl solution with and without TBE as an inhibitor. The IE% obtained from EIS results were almost similar to the PP analysis results and confirmed it. The EIS plots showed that the increment of TBE concentration leads to the increment of  $R_p$  (charge transfer resistance of aggressive ions i.e., Cl<sup>-</sup> to the copper surface) which is predictable and refers to the formation of a thin and protective layer of TBE molecules on the copper surface leading to the reduction of Cl<sup>-</sup> attack to the surface resulting from the reduction of copper dissolution and inhibition improvement. The temperature effect on the corrosion rate of copper in the presence and absence of TBE has been evaluated in several temperatures from 298 to 338 K and it was confirmed that increasing the temperature leads to the corrosion rate increment. Finally, SEM-EDS and GC-MS analysis have been utilized to evaluate the copper surface changes and to find the chemical composition of TBE, respectively.

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