ABSTRACT BOOK

10th National Seminar (Webinar) of Chemistry and Environment

1 - 2 November, 2021

Department of Chemical Engineering
Faculty of Engineering
Quchan University of Technology

10th National Biennial Seminar
of Chemistry & Environment

Iranian Chemical Society

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Prepared by:

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Conference President,
Quchan University of Technology,
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Welcome Message

from the Conference President

Dear scholars, researchers, and guests, I shall first thank the Almighty for the honor bestowed upon me to convey my greetings and respect to you on this very occasion, the scientific gathering for the 10th national Biennial Seminar (Webinar) of Chemistry and Environment, to review the most advanced measures in the field of chemistry & environment, which will be held in the Quchan University of Technology, Quchan, Iran. Over the years, significant developments in agriculture, energy, and health have been developed that have contributed to human well-being. However, some of these improvements in our lives have resulted in changes to the environment around us.

Our environment is a hugely complex system that includes the air we breathe, the land we live on, the water we drink, and the climate around us. It must be work to ensure that our developments in some areas do not adversely affect our environment whilst also ensuring that we mitigate any damage that has occurred. Work by some researchers has shown that we are already at a tipping point that might lead to "non-linear, abrupt environmental change within continental- to planetary-scale systems".

As we strive towards a better world, we work to ensure chemistry's contributions are realised. Chemistry can help us to understand, monitor, protect and improve the environment around us. Chemists are developing tools and techniques to make sure that we can see and measure air and water pollution. They have helped to build the evidence that shows how our climate has changed over time. And they can be part of the effort to understand and address new problems that we face like microplastics and the potential effects of the different chemicals that we are exposed to.

With profound gratitude to the organizers of this event, it is my fervent wish that during this conference we can create a suitable atmosphere to present the achievements of researchers and intellectuals as well as discussing and exchanging views with the aim of promoting sustainable development of science.

I hope that, with the will of God Almighty and the complete eradication of the coronavirus transmission chain, you will honor us with your presence in the Quchan in the foreseeable future.

May God bless all with good health and prosperity.

Dr. Ali Asghar Beheshti
President of Quchan University of Technology

Associated Professor of Chemistry,
Department of Chemical
Engineering,
Faculty of Engineering,
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Quchan, P.O. Box 94771-67335,
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Welcome Message

from the Conference Scientific Chair

On behalf of the organizing committee, I am honored and delighted to welcome you to the 10th national Biennial Seminar (Webinar) of Chemistry and Environment. This seminar is among the leading scientific events, gathering researchers and specialists from academia and industry to share their latest research headways and achievements in the field of chemistry and environment. The Quchan University of Technology is honored to host the 10th national Biennial Seminar (Webinar) of Chemistry and Environment during Nov. 1&2- 2021. Due to the Covid-19 pandemic and for the safety of participants, this year's conference will be conducted.

The 10th national Biennial Seminar (Webinar) of Chemistry and Environment covers a uniquely wide scope of related topics including Air, Water, Soil, Waste Management and Recycling, Education & Environment, COVID-19 & Environment, Clean Fuels, Nanotechnology, Renewable Energy, Chemometrics, Green Chemistry, Environmental Standards, Groundwater pollution in Quchan.

The comprehensive range of sessions provides a special opportunity for students, academic scientists, researchers, and industry representatives to exchange their latest innovations and finding, get useful comments on their work, build collaboration and establish contacts. The scientific program is going to be diverse with interesting keynote speeches and invited talks as well as oral and poster sessions.

The organizers are looking forward meeting all of you in the 10th national Biennial Seminar (Webinar) of Chemistry and Environment.

Once again I am delighted to invite you all to take part in this conference and also to make the conference a grand success.

Thank you for your participation in 10th national Biennial Seminar (Webinar) of Chemistry and Environment.

Yours Sincerely,

Congress Scientific Chair
Tahereh Rohani Bastami, Ph. D.
Associated Professor of Chemistry,
Department of Chemical Engineering,
Faculty of Engineering,
Quchan University of Technology,
Quchan, P.O. Box 94771-67335, I.R. IRAN

T. Rohani. B.

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Keynote Speakers

The Unexpected Cosequences of Environmental Manioulations

I. Yavari

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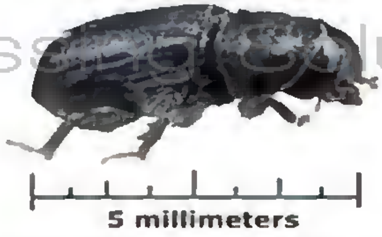
Frequently, the environmental manipulations leads to unexpected problems. Two cases will be discussed: (a) From 1940s to 1980, DDT was extensively used in agriculture and it has been estimated that a total of 1.8 million tonnes have been produced and used globally. DDT is a persistent organic pollutant that is readily adsorbed to soils and sediments, which can act as long-term sources of exposure affecting organisms; and (b) Dutch elm disease devastated elms throughout Europe and North America in the second half of the 20th century. Multistriatin is a pheromone of the elm bark beetle, which has been effectively used against elm bark beetle. Some Iranian environmental issues will be presented and discussed.

DDT



Elm Bark Beetle

Microplastics and Effects on Aquatic Ecosystems

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Microplastics (MPs) are reconsidered as a major concern over the past decade due to their defined harmful effects to ecosystem and human health. The Persian Gulf is characterized to the leading oil producer in the world, high estimates of solid waste generation, especially plastics. In Persian Gulf, some reports have been investigated the concentrations of MPs, their distribution, risk assessment, transfer during food webs, their quantitative and qualitative characteristics in sediments, marine organisms and to a lesser extent, wastewater outlets. The findings of previous studies indicated the most MPs are fibers and fragments polyethylene (PE) and polypropylene (PP) with dominants colors white, black. However, up to date, there are not reports to assess MPs of wastewaters during the refining process. Here, this study was performed to assess the distribution and quantitative and qualitative measurement of MPs in sewage effluent entering the treatment plant of Bandar Abbas for the first time. Deep and surface water sampling was performed monthly and seasonally, respectively, from five stations in the range of wastewater inlet to wastewater outlet from refinery of Bandar Abbas. The samples were filtered through 500, 300, 100 and 30 µm sieves. The MPs were isolated by hydrogen peroxide digestion and subsequent density separation using NaCl solution. The finding of the concentration of MPs in deep and surface waters indicated the dominant MPs of sewage inlet station are >500 and 300-500 µm in size during spring to winter, respectively. The maximum reduction of MPs>500 and 300-500 µm was observed in fourth station during spring to winter, respectively[2]. The most commonly recovered polymers were polyethylene (PE) and polypropylene (PP) in all size classes. This study provided comprehensive assessment of MPs during the refining process for the first time. Further detailed field investigations are required to better understanding the distribution and source of MPs in this region.

Application of Nanosorbents for Separation of Environmental Pollutants in Food

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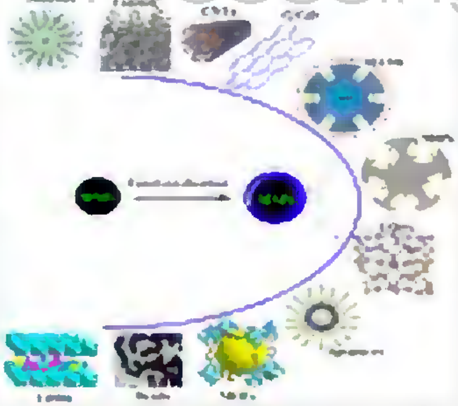
In the last years, nanotechnology progress has impacted several fields of food science. In food analysis, new nanomaterials have been developed in order to extract minority food components. Recently, magnetic nanoparticles (MNPs) have been used as sorbents in methodologies several fields of food science. Nowadays, magnetic sorbents, especially nanostructured ones, are widely used in sample preparation techniques as well as for removal of pollutants from the environment. Application of magnetic sorbents considerably simplifies the sample pretreatment process without filtering and centrifugation as well as ease recycle and reuse of the sorbent. Magnetic sorbents such as NPs, nanocomposites are generally used for preconcentration purposes. However, sponges, foams, hydrogel, and beads are generally used for removal purposes. Synthesis of novel magnetic hybrid sorbents by using advanced nanostructured materials such as MOFs, LDHs, G/GO, CNTs, COFs, RAM, MIPs and aptamers are being developed to find more efficient sorbents and introduce different extraction mechanisms at the same time.



Electrochemical Immunosensors in Environmental and Clinical Analysis: Current status, Challenges, and Perspectives

H. Bagheri

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Immunosensors are one of the most important classes of affinity biosensors based on the specific recognition of antigens by antibodies to form a stable complex, in a similar way to immunoassay. The development of electrochemical immunosensors towards clinical and environmental detections has been in the spotlight for several decades. Also, the publications in this field have grown exponentially over the past decades, making it a trending hot-spot. Due to the limitations of conventional analytical methods and the wide perspective of point, the immunosensors are as promising candidate with the critical aspects that require great attention in order to fulfill the criteria of biomedical diagnostics, food safety control, and environmental monitoring will be covered. Electrochemical detection holds the broader applications in different fields of sensing and biosensing because it has several advantages such as sensitive, fast, simple, portable and low-cost. In addition, multiplexing capability for simultaneous detection of multiple analytes is feasible. Unfortunately, transition of biosensors from laboratories to the market is challenging. In this presentation, I will present recent advances and discuss the ongoing challenges and future opportunities associated with detection based on electrochemical immunosensors for human health that include specific disease markers, individualized diagnosis of cancer subtypes, therapeutic and addictive drugs, food residues, and environmental contaminants.

Investigating The Relationship Between Urmia Lake Rehabilitation Program and The lake Brine Chemistry Variation

1. R. Lak, 2. A. Mohammadi, 3. J. Darvishi Khatouni

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Iran with dry and semi-dry climatic characteristics and a relatively low annual precipitation contains several saline's and hypersaline lakes with different sizes and shapes. These lakes from the environmental, past climate, geological and geographical points of view are unique and important settings. In the last two decades, Urmia lake as the second large hypersaline lake in the world, due to human mismanagement experienced an extremely rapid water level fall (>6 m) which threatens several millions of people around the lake who are settled down in several large and small cities. Therefore, the preservation and revitalization of Urmia Lake are very important in terms of natural and social hazard management. Aware of that, the Urmia Lake rehabilitation program without lake brine chemistry monitoring in the dry and wet seasons is not able to understand and predict the future behavior of this water body, we have measured the lake water Physico-chemical parameters and ionic composition in the last 12 years (the time period between 2008 to 2019). The Physico-chemical parameters including water depth, water salinity, density, temperature, pH, EC, and TDS were measured during field works in both wet and dry seasons and the lake water ionic composition (Na+, K+, Mg2+, Ca2+, Cl-, SO42-, CO32-, HCO3-) were measured. Our results indicate that the lake water ionic composition and Physico-chemical parameters are rapidly varying from wet seasons to dry seasons. In the dry condition due to decreasing lake water input and continuous evaporation, the amount of all ions in the lake water and consequently lake salinity is increasing. This leads to the deposition of evaporite minerals (dominantly halite > 98%) as a salt crust in the lake floor. Deposition of halite leading to egress of Na+ and Cl- from the lake brine and consequently increasing of Mg2+ and Ca2+ cations of lake water which affects the lake brine type. For a long time, the Urmia lake water brine type was Na-Mg-Cl until 2008. In the time periods between 2009-2018 due to extreme water level fall and thick salt crust deposition, the lake brine type changed to Mg-Na-Cl and since 2019 due to increase of freshwater input to the lake and slight lake water level rise, the brine type again changed to Na-Mg-Cl (similar to before 2008). In fact, the rehabilitation programs of Urmia Lake leading to the revival of lake brine chemistry. However, the present lake brine chemistry and type is in an unstable condition. Therefore, maintain the current conditions of the lake depend on the balance between water input and output from the lake.

Conversion of Carbon Dioxide to Fuels and Chemicals

Prof. Shuguang Deng

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Anthropogenic emissions of carbon dioxide from industrial processes including energy production are considered the major cause of global warming and ocean acidification. Massive abatement strategies on carbon capture and sequestration are being developed to solve this urgent environmental problem. However, the existing carbon capture and sequestration approach is not sustainable because carbon dioxide emitted from industrial processes is considered a liability, not a resource. A more sustainable strategy is to convert the captured carbon dioxide into fuels and chemicals rather than sequestering the carbon underground. This presentation will discuss the recent developments and future perspectives in carbon dioxide utilization for the sustainable production of fuels and chemicals and mitigation of global warming. Carbon dioxide can be converted into value-added products through hydrogenation, esterification, methanation, reforming, and reverse water-gas shift reactions. Examples of selective CO2 electroreduction on single-atom copper catalysts developed in our lab most recently will be discussed in detail in this presentation.

A Review of Heavy Metal Contamination Indices Assessment in Soil

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In recent years, various human activities such as the rapid urban development, agriculture and the increase of industries have caused environmental pollution with heavy metals. Heavy metals create significant potential risks for body of living organisms, especially humans. Therefore, measuring them in nature has become an important to control resources and reduce their harmful effects. Multiple pollution indices can be used to quantify the anthropogenic influences heavy metals pollution in soil. Different pollution indices, such as Enrichment factor (EF), Geoaccumulation index (Igeo), Nemerow's integrated pollution index (NIPI), Contamination factor (Cf), Pollution load index (PLI), Potential contamination index (PCI), Modified pollution index (m-HPI), Ecological risk factor (Er), and Potential ecological risk index (PER) has been introduced for analytical evaluation of contamination. These quantitative indices demonstrate heavy metal pollution in the studied area and it can be used by national department of environment to announce risk status, provide a relative ranking of pollution and their management. Due to the risk of pathogenicity and carcinogenicity of heavy metals, non-carcinogenic and carcinogenic risk indices have been considered by many researchers are widely used to assess the risk to human health.

Oral Presentation

Aqueous Photooxidation of 1,5-Dihydroxynaphthalene to Juglone Under Heterogeneous Conditions

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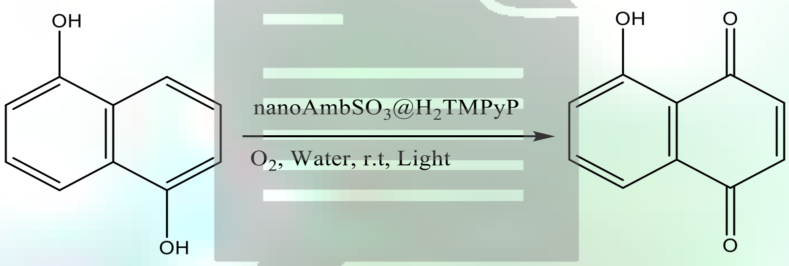
Graphical Abstract



Abstract: Aerobic photooxidation of 1,5-dihydroxynaphthalene in water and the presence of a cationic porphyrin immobilized into the pores of a nanostructured mesoporous polymer is reported.

Phenolic compounds are considered as the main organic water pollutants with strong toxic effects even at very low concentrations.[1] Photooxidation of 1,5-dihydroxynaphthalene (DHN) as a representative compound of polyphenols series in the presence of various photosensitizers, has been the subject of extensive studies.[2,3] The design of new photosensitizers with high photocatalytic activity and oxidative stability has been of great interest for many applications.[4] In the present study, a *meso*-tetra(aryl)porphyrin with cationic *meso* substituents, *meso*-tetrakis(N-methylpyridinium-3-yl)porphyrin (H_2TMPyP), immobilized on a nanostructured cation exchange polymer, amberlyst 15, nanoAmb was used as a photosensitizer for short time photooxidation of DHN to Juglone at room temperature. As an important therapeutic phytochemical, Juglone has many applications as in textile, food and cosmetic industries as a natural colorants [4]. The synthesis and characterization of the nano-structured polymer, the corresponding sodium salt and the polymer supported porphyrin were explained elsewhere. [5,6] The photooxidation of DHN was conducted in water in the presence of 10 W white LED lamp, using the photosensitizer (nanoAmbSO$_3$@H$_2$TMPyP) and DHN in a 1:10 molar ratio. The oxidation reaction was monitored by UV-vis spectrophotometry at the λ_{max} of DHN and Juglone, 301 nm (ε = 7664 M^{-1} cm^{-1}) and 427 nm (ε = 3811 M^{-1} cm^{-1}), respectively. The oxidation was completed in 60 s (Figure 1). No catalyst degradation was observed in the short reaction time used for the oxidation of DHN.

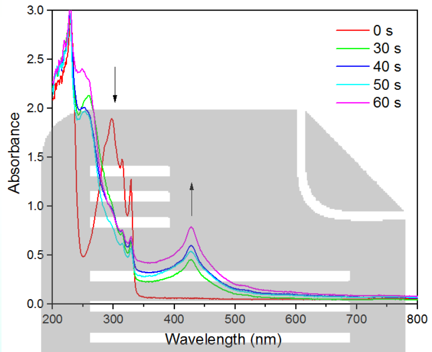


Figure 1. Aerobic photooxidation of DHN catalyzed by nanoAmbSO$_3$@H$_2$TMPyP in water.

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Designing a Template By 3D Printer for Construction of Lab-on-Paper Chemical Sensor Containing Silver Nanoparticles for The Measurement of Thiosulfate in Water Samples Using Smartphone

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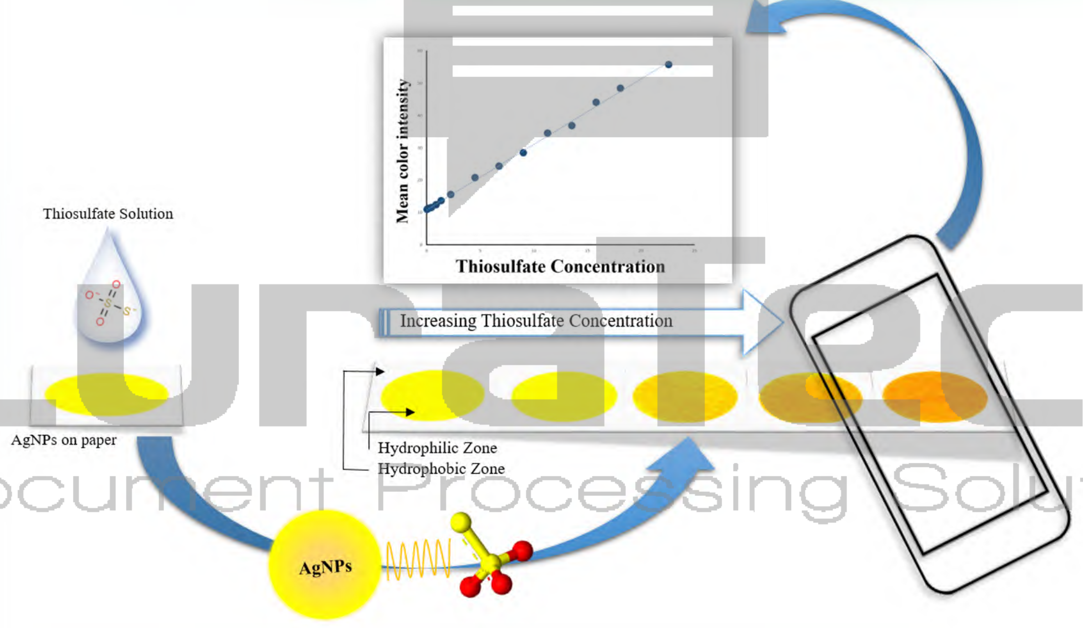

Abstract: The chemical sensors are laboratory equipment that play important role in environmental, chemical, and biological measurements, and have become smaller in size and dimensions called lab-on-chip devices [1]. Many features such as small size, biodegradability, and ability to use micro volumes samples in the detection zone of analysis have made the paper as a substrate for such sensors [2]. The basis of paper based analytical devices (PAD) and also lab-on-paper was introduced by Whiteside et al. [3]. In this research, we designed a template for the construction of lab-on-paper chemical sensors containing silver nanoparticles for measurement of thiosulfate ion in aqueous solutions. We designed a pattern in solid works

software and then printed the template in the 3D printer device, and used it to make PADs by wax dipping method, which resulted in PADs with good performance. The detection zones of PADs containing silver nanoparticle (AgNPs) are yellow but in the presence of different concentrations of thiosulfate ions turn red because of the interaction of AgNPs and thiosulfate ion and are darker at higher concentrations of thiosulfate. The detection zones are photographed and the mean color intensity of the zones is determined in Photoshop software. These color intensity changes were used as analytical signals for the determination of thiosulfate. The experimental conditions such as synthesis of AgNPs, sodium hydroxide concentration, number of injecting AgNPs on the paper were optimized to achieve maximum analytical signals. By applying the optimal conditions, a linear calibration graph in the range of 0.05-22.60 µg mL^{-1} was obtained and the limit of detection was 0.025 µg mL^{-1}. The relative standard deviation (RSD) for 8 replicate measurements of 0.23 and 4.52 µg mL^{-1} were 4.17 and 2.20, respectively. This system was used to determine thiosulfate in water and wastewater samples with good recoveries.

Reference

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Prediction of Biological Activities of Some Pesticides by QSAR Method and Molecular Docking Study

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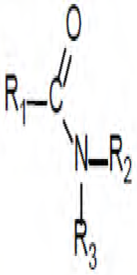
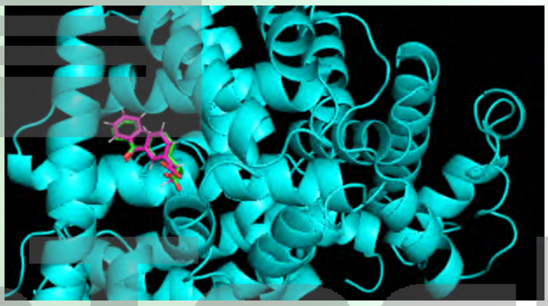
Graphical Abstract





Abstract: In the present study, the toxicity dose of some pesticides (LD50) was modeled and predicted using quantitative structure-activity (QSAR) and molecular docking studies. In the first part of this study, the aim is to present a QSAR model for predicting and calculating the toxicity dose of pesticides. For this purpose, after calculating the molecular descriptors, multiple linear regression (MLR) and genetic algorithm (GA) methods were used to select the best descriptors related to the toxicity dose of these compounds. Then selective descriptors were used as inputs to build linear (MLR) and nonlinear support vector machine (SVM) models. By comparing the results, this result was obtained that the nonlinear MLR-SVM model had best R and SE values. R and SE values for the training set are equal to 0.99 and 0.014 and for the test set equal to 0.718 and 0.082, respectively. In the second part of the study, pesticides with the highest and lowest levels of toxicity were studied by molecular docking studies. Compounds No. 35 and 63 with the lowest toxicity with LD 50 are equal to 2.21 and combination 57 with the highest toxicity with LD 50 is equal to 2.68. Obtained result was concluded that compounds that tend to form more hydrophobic bonds are more active and cause more toxicity, and also the presence of some elements such as fluoride increases the

toxicity of compounds. Selected descriptors and correlation between them are shown in table 1 and 2, respectively.

Table 1

No.	Descriptors
V_1	SaasC
V_2	mindO
V_3	nHBa
V_4	GATS3i
V_5	AATS8i
V_6	GATS5m
V_7	nsssN
V_8	MDEC-33

Table 2

	V1	V2	V3	V4	V5	V6	V7	V8
V1	1	.098	-.224	.220	-.004	-.420	.202	-.055
V2		1	.199	.055	.063	-.142	.341	.360
V3			1	-.061	.208	-.208	-.172	.594
V4				1	-.134	-.227	.148	.076
V5					1	-.108	.034	.037
V6						1	-.188	-.277
V7							1	-.156
V8								1

y-scrambling and sensitive analysis are in the table 3 and figure 1, respectively.

Figure 1

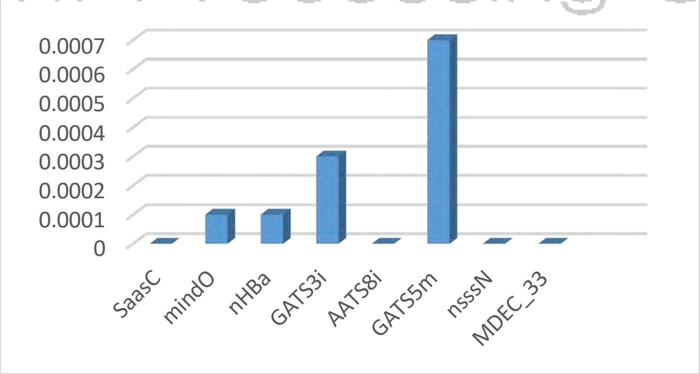


Table 2

Q2	No.	Q2	No.
0/321	11	-1/857	1
-0/719	12	-1/196	2
-1/272	13	-2/444	3
0/305	14	-0/791	4
-3/476	15	-3/197	5
0/836	16	-1/516	6
-0/76	17	-0/242	7
-1/16	18	-1/45	8
-0/00062	19	-1/111	9
-3/056	20	-0/209	10

The toxicity data range is from 2.21 to 2.62, of which data 35 was selected as the weakest and data 57 as the strongest toxicity effect for the docking study.The crystal structure of albumin in complex with ketoprofen with code 6 OCK is shown in Figure 2, which is taken from the protein database in PDB format. This protein with a resolution of 1.90 angstroms and an R value of 0.192 was selected as the appropriate protein model.

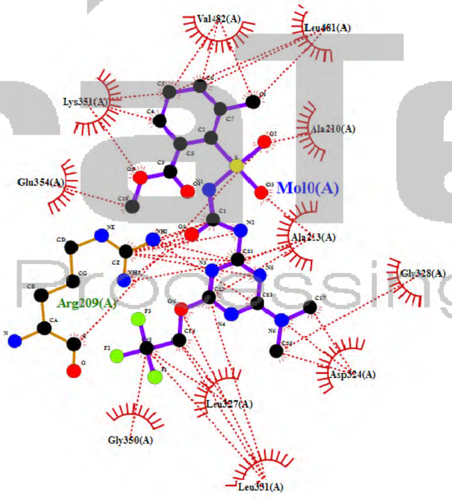


Figure 2

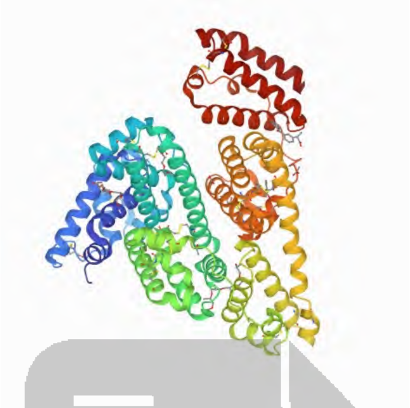


Figure 3

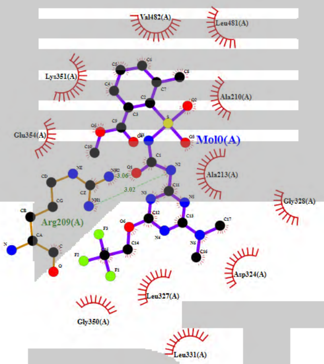


Figure 4

Two-dimensional design of Ligplt software on hydrogen and hydrophobic bond interactions between compound 57 and serum albumin amino acids were shown in figure 3 and 4, respectively. As shown in these figures, Composition 57 has 12 interactions with the albumin binding site. Binding amino acids include Leu481, Val482, Lys351, Glu354, Arg209, Gly350, Leu331, Leu327, Asp324, Gly328, Ala213, Ala210, that Leu481, Val482, Lys351, Glu354, Glu350, Gly350 Leu327, Asp324, Gly328, Ala213, Ala210 have hydrophobic interactions with compound 57, while Arg209 interacts with this compound through hydrogen bonding. Molecules like compound 57 that are more capable of making hydrophobic bonds are more active and have a greater toxicity effect. Also, according to the structure of this compound, it can be concluded that the presence of elements such as fluorine increases toxicity.

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Study on Adsorption of Dibenzothiophene by Cu-Immobilized Alginate Adsorbent from Diesel Fuel

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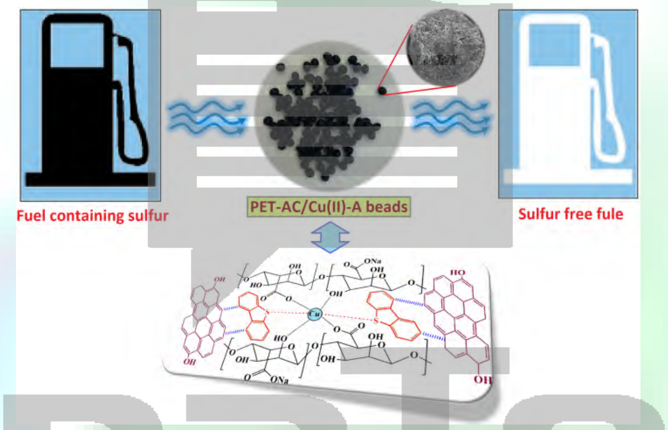
Graphical Abstract



Abstract: With the increase of the urbanization and industrialization, the consumption of fossil fuels is also gradually increasing. These fuels essentially includes large concentrations of sulfur compounds which produce hazardous oxides such as SOx during combustion, causing significant serious environmental pollution [1]. Accordingly, efficient removal of organosulfur compounds like thiophene (T), benzothiophene (BT) and dibenzothiophene (DBT) from gasoline and diesel fuel is a hot topic of research [2, 3]. In this study, adsorption of DBT on copper(II)-alginate (Cu(II)-A) beads containing sustainable PET-AC investigated. The choice of Cu(II) is based on the expected higher affinity for organosulfur molecules and economic point of view. Structural and surface properties of PET-AC/Cu(II)-A beads were analyzed by Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray (EDX) analyzer and N_2 adsorption-desorption test. DBT adsorption ability of the

fabricated adsorbent beads was studied by static adsorption experiments. The effects of PET-AC mass ratio in Cu(II)-A beads on the surface area and desulfurization efficiency were studied. The adsorption kinetics, adsorption isotherms, thermodynamic parameters and adsorbent reusability were also researched. The adsorption isotherms could be correlated by the Langmuir isotherm and the maximum adsorption capacity reached up to 62.9 mg g^{-1}. The study of kinetic parameters showed that the DBT removal had followed a pseudo-second order kinetic model. Lewis acid-base and π–π interactions might be the driving force of the desulfurization process. The adsorbent could be also reused for 4 successive runs with negligible loss in desulfurization capability. All of these features make the PET-AC/Cu(II)-A as a potential adsorbent towards desulfurization from fuels.

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Investigation of Self-Healing Properties of Nanocomposite Polymer-Modified Natural Hydrogels

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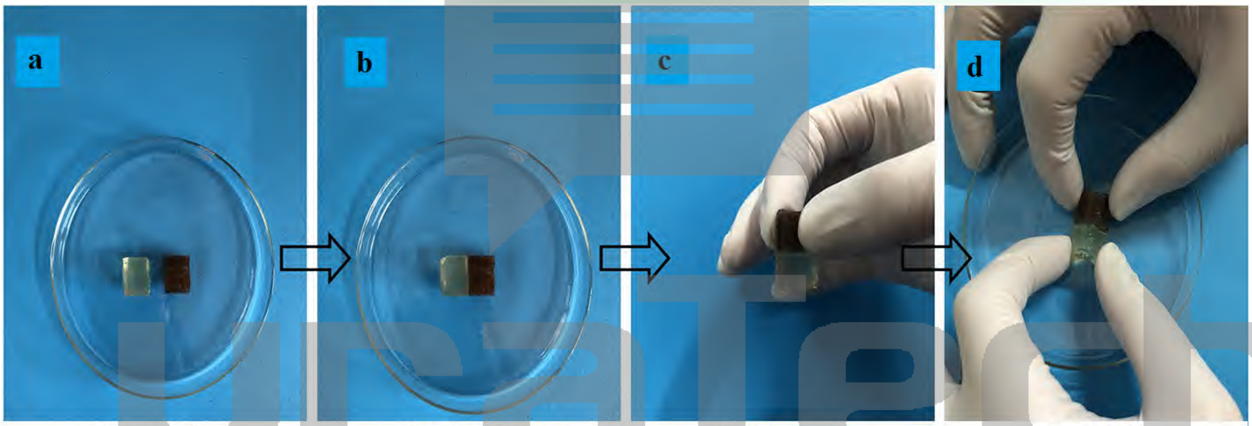
Graphical Abstract



Hydrogel pieces Put together Healed after 2 h Stretched

Hydrogel pieces with Fe3O4 nanoparticles Put Magnet Healed after 10 min

Abstract: Recently, the use of nanocomposite hydrogels that can repair small cracks caused by various external stresses has been considered. [1] Self-healing property refers to the ability of a substance to repair damage and restore original function inherently or non-intrinsically. [2]

In this study, natural hydrophilic materials such as gelatin and salep were used as the primary material to prepare hydrogels. To improve the properties of the hydrogel, the Reversible Addition Fragmentation Polymerization method (RAFT) was used to modify the hydrogel, and finally synthesized Fe_3O_4 magnetic nanoparticles [3] was incorporated into the matrix to prepare hydrogel

nanocomposites that have self-healing properties. The use of Fe_3O_4 nanoparticles and synthetic polymer not only improves the mechanical properties of nanocomposites but also makes them efficient in some applications like adsorbents and smart biomaterials. [4]

The structure of the synthesized hydrogels was characterized by FTIR, FESEM, XRD, and EDAX analysis. The self-healing properties of hydrogels were investigated by making incisions and placing them under a magnetic field. The swelling rate of synthetic hydrogels in acidic, alkaline, and neutral conditions was investigated by changing the amount of crosslinking agent and different amounts of synthesized nanoparticles. The addition of synthetic nanoparticles to the structure of hydrogels increased structural strength, improved swelling, and self-healing properties.

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The Remarkable Activity of Fe-NC/S,N,CNTin ORR for Passive Direct Ethanol Anion-Exchange Membrane Fuel Cells

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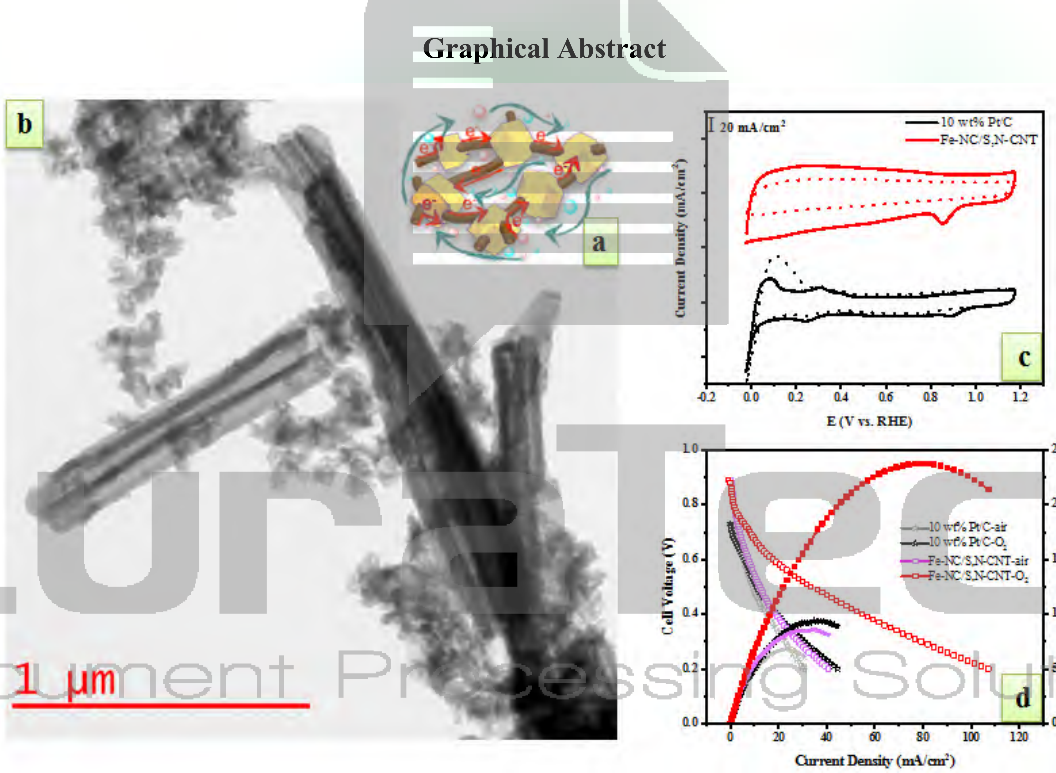

Fig1. (a)Graphical Abstract,(b)HRTEM image, (c) CV plots at 10 mV.s^{-1} in 0.1 M KOH solution saturated with N_2 and O_2, (d) The alkaline DEFC performanceat room temperature with Fe-CN/ S,N-CNs (2.0 mg$_{metal}$/cm^2) and 10wt% Pt/C (2 mg$_{Pt}$/cm^2) used as the cathode. The anode used was 60wt% Pt/C (20 mg$_{Pt}$/cm^2) with 2 mol/L CH_3CH_2OH in 2 mol/L KOH supplied as fuel. The air and O_2 was supplied to the cathode without flow rate.

Abstract: In recent decades, Portable direct ethanol fuel cells (DEFCs) have been considered as renewable and environment-friendly energy sources due to their higher volumetric energy density, lower costs, higher safety, ease of storage and transportation in fuel utilization [1-3]. Thus it is necessary to use an active,

nonprecious and ethanol-tolerance catalyst to minimize the losses in power density and energy efficiency [4, 5]. *Therefore, the production of electrocatalyst with the optimized percentage of metals and suitable nitrogen and sulfur doping level enable control of their properties to enhance their performance.* Thereupon, composite MOF-polymer (Fe-ZIF-PPY) was carbonized under argon atmosphere and finally, nanocomposite (Fe-NC/S,N,CNT) was obtained (Fig a). The electrocatalytic property, structure and morphology of Fe-NC/S,N,CNT were explored via various characterization techniques (Fig b). Applicability of the S-doped Fe-N-C catalyst in alkaline media was exhibited very high ORR activity (Fig c)with half-wave potential at 1.0 V (vs. RHE)*and the Tafel slope of 53 mV/dec* which satisfactory results were achieved. Also, in anion exchange membrane direct ethanol fuel cell (AEMFC) under identical conditions, two cathode made with this optimize electrocatalyst and Pt/C and power density were obtained in 25 mW cm^{-2} at 0.6 V and 9 mW cm^{-2} respectively (Fig d). based on the obtained results, the performance of Fe-NC/S,N-CNT catalyst was assessed optimum in DEFC. As structural properties such as the specific surface area, porosity, and high density of active site have important roles in boosting this performance.

Keywords: Direct Ethanol fuel cell, Anion-exchange membrane, Metal-organic Frameworks, Cathode Catalysts.

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P. G. Santori, F. D. Speck, S. Cherevko, H. A. Firouzjaie, X. Peng, W. E. Mustain and F. Jaouen, ***Journal of The Electrochemical Society***, **167**, 134505, **2020**

Synthesis of Nitrogen-Doped Carbon Dots from Natural Material for Fluorometric Determination of Cr(VI) in Industrial Waste, Drinking Water and Serum Samples

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Graphical Abstract

Abstract: Chromium enters the environment as a result of effluent discharge from different industries, including electroplating, steel, tanning, and oxidative dyeing, and water cooling towers. The toxicity of chromium is a function of the concentration and its oxidation [1]. Cr(III) is essential for living organisms especially human beings, while Cr(VI) is known as a toxic species that can easily penetrate the cell wall and exert its noxious influence in the cell. Cr(VI) is also known as a cause of different cancer diseases [2]. Therefore, the development of sensitive and fast analytical methods for accurate and selective determination of Cr(VI) is important [3].

In this study, nitrogen-doped carbon dots (N-CDs) were synthesized by one-pot microwave treatment of Ranunculus farsicus leaves extract as the carbon source and urea as the nitrogen source and applied as a fluorimetric nanosensor for selective and sensitive determination of Cr(VI)

ions. The N-CDs have a relatively uniform size of approximately 5.6 nm and good water dispersibility. The N-CDs exhibit strong visible fluorescence and high stability at pH 7.0. The fluorescence intensity of the N-CDs would be turned off in the presence of Cr(VI) ions by the mechanism of the inner filter effect (IFT). The limit of detection for Cr(VI) was found to be 0.750 μM and the relative standard deviation (RSD) at 100.0 μM of Cr(VI) was 5.6% (n = 5). The proposed method was successfully applied for the determination of Cr(VI) industrial waste, drinking water, and serum samples.

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Investigation of ZIF-67 and ZIF-67-NH2 as Catalysts for Biodiesel Production

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Abstract: Due to global warming and the origin of its fossil fuels, researchers have put the production of clean fuels on the agenda. In this paper, biodiesel fuel was produced using ZIF-67 and ZIF-67-NH2 catalysts, which are from the family of organic metal frames and have good catalytic properties. This fuel is a suitable alternative to oil and gas fuel. In this study, fuel production was optimized at the temperature and ratio of oil to alcohol and the time and amount of catalyst, and BET-FT-IR and XRD analyzes were performed. The optimum conversion percentage for ZIF-67-NH2 catalyst is 0.01 g at 60 ° C and the ratio of methanol to oil is 20 in 40 minutes.

Photocatalytic Degradation of Malachite Green (MG) Dye Under UV Light Irradiation by Zr/CeO2 Nanocomposite

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Abstract: Textile industries has a significant impact on the environment due to produce of huge expending of synthetic dyes. Besides, due to large consumption of water and large amounts of processed dye effluents, it is necessary to treat of such wastewaters. Malachite green is an organic compound that is used as a dye for silk, leather, and paper and is carcinogenic, mutagenic, chromosomes breaker and toxic to mammals. In this research, Zr/CeO2 nanocomposite was synthesized via ultrasonic and was characterized by FTIR, XRD, FESEM, EDS, and TEM, UV-Vis, PL and DRS techniques. Then, efficiency of synthesized Zr/CeO2 nanocomposite was studied for photocatalytic degradation of malachite green (MG) dye under UV light irradiation (300 watt). However, effect of Zr/CeO2 nanocomposite dosage, initial pH of solution, initial malachite green concentration and irradiation time was investigated on photocatalytic degradation of malachite green dye. Results show that malachite green dye degradation was achieved equilibrium within 45 min. According to the results, 80.18% of malachite green degradation was obtained at [MG]=20 mg/L ,Zr/CeO2 dosage=0.05g /50mL, pH =10 and irradiation time = 45 min conditions. Also, the kinetic of photocatalytic degradation of malachite green was investigated and results revealed that photocatalytic degradation of malachite green is obeyed pseudo-second order kinetic model. Thermodynamic studies were calculated for the photocatalytic degradation of malachite green by Zr/CeO2 nanocomposite and the results indicated exothermic nature and non-spontaneity of the process. Overall, as a results Zr/CeO2 nanocomposite has a great potential to photocatalytic degradation of malachite green from aqueous solutions under UV light.

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Occurrence and Abundance of Microplastics in Offshore Sediments of The Persian Gulf and Gulf of Oman

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Graphical Abstract

Abstract: Plastic materials are trackable in every corner of our biosphere [1]. Some of these materials are intentionally designed to be very small and the others gradually break down into what we know as Micro-plastics (MPs). These tiny plastic bits are < 5 mm in all dimensions, but they are also the most prevalent form of plastic pollution observed on the Earth [2]. A lot of the MPs finally reach and gradually deposit into the marine sediments. By doing so, the MP bits act like miniature "Trojan horses", delivering toxic chemicals to the aquatic animals because of inadvertent intake [3]. The Persian Gulf is a young body of water continually supported by the budget of Oceanic waters of the Indian Ocean, entering through the Gulf of Oman. Since the Persian Gulf is a semi enclosed and shallow region, increasing human activities would result in deleterious repercussions. This is a matter of concern especially in the case of marine debris having recalcitrant nature, notably MPs. By now, no valid report from Offshore Micro-plastics in the sediments

from ROPME region (The Persian Gulf and the Gulf of Oman) has been published despite an increasing impetus in marine MPs related surveys. It was thus the topic of a widespread sampling, scheduled in marine expedition of the PERSIANGULF Explorer in 2019. In sum, 51 stations were sampled and subjected to further analysis including MPs content (particles Kg^{-1}), physical features and spatial distribution. The finding demonstrated that the density of MPs varies from stations with minimum number of 5 to a single station with a maximum number of 75 particles Kg^{-1}. The dominant shape of extracted MPs was fiber and it was in a good agreement with the findings that the fibrous particles are prevalent form of MPs in the marine environments. According to the results, Black fibers were the dominant colored particles detected and the white ones share a minimal part. The majority of fibers (39%) possessed a size range of 0.5 to 1 millimeter and the size limit detected was something about 100 micrometers. Correlation analysis was run to distinguish any possible dependency among density of MPs and grain-size, organic matter and distance of sampling points from the mainland. The analysis revealed that the density of MPs is not a correlate factor of grain size, organic matter and distance from the mainland.

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Comparison of Co/Zn-NC@PPy-800 and Commercial Pt/C as the Cathode Electrocatalyst of Fuel Cell-based Breath Ethanol Sensor

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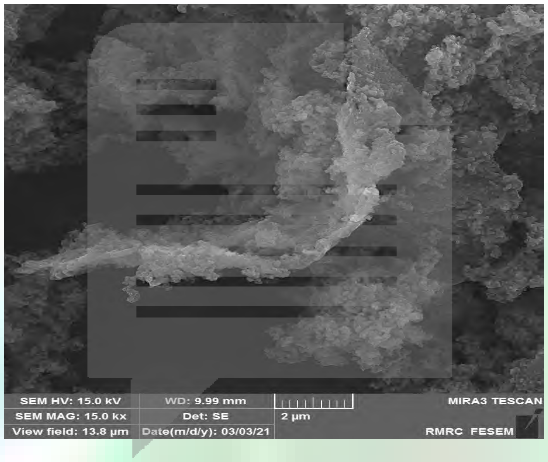

Fig1. SEM image of Co/Zn-NC@PPy-800

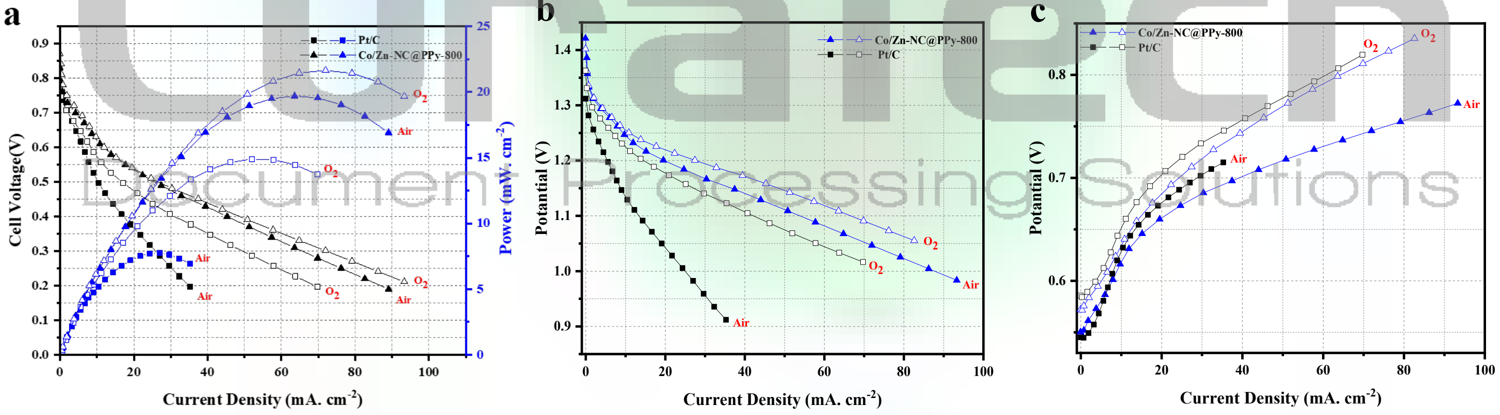

Fig2. (a) V-i-P curves, (b) cathode and (c) anode polarization curves of air breathing direct ethanol fuel cell with Co/Zn-NC@PPy-800 and the commercial 10 wt.% Pt/C as the cathode in 2 M ethanol in 2 M KOH.

Abstract: Alkaline direct ethanol fuel cells (DEFC), which convert the chemical energy stored in ethanol directly into electricity, are one of the most promising energy-conversion devices for portable, mobile and stationary power applications as well as highly sensitive devices for ethanol sensing.

Exploring highly active, stable, and inexpensive electrocatalysts for the oxygen reduction reaction (ORR) is pivotal in developing sensitive sensors. In this research, synthesized Co/Zn-NC@PPy-800 and commercial Pt/C are used as ORR catalyst. In the SEM image (Fig. 1), Co/Zn-NC@PPy-800 NPs on the polypyrrole sheets are formed N-doped nanosheet-like carbon. The fuel cell performance curves are shown in Fig. 2. Two identical cells are made using the same anodes and Co/Zn-NC@PPy-800 and commercial 10 wt.% Pt/C as the ORR electrocatalyst for cathode fabrication. The anion-exchange membrane (A201 Tokuyama), with a thickness of 28 μm is used as electrolyte. 2 M of ethanol in a 2 M KOH solution which was stabled in 12 ml tank was fed to the anode side and cathode was performed under air breathing and O_2 bleeding modes. In fig. 2a, polarization and power density curves are displayed and explaining the fuel cell has better performance when it equipped with Co/Zn-NC@PPy-800 in compare with 10 wt. % Pt/C as cathode catalyst. Furthermore, using non-noble synthesized cathode catalyst, the I-V behavior shows no significant change under O_2 and air breathing modes. The cathode polarizations are depicted in fig. 2b. It can be seen that Co/Zn-NC@PPy-800 is more active than 10 wt. % Pt/C for ORR in both O_2 and air breathing modes which means Co/Zn-NC@PPy-800 has better tolerance against ethanol crossover in compare with 10 wt. % Pt/C. In addition, according to the Fig. 2c, the cell polarization curve in Co/Zn-NC@PPy-800 case is only depends on anode polarization and oxygen partial pressure in oxidant flow has no effect on fuel cell response.

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Deoxygenation and Acidification of The Persian Gulf in A Changing Climate

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Abstract: Dissolved oxygen (DO) concentrations in coastal areas have been decreasing in many regions over the past decades mainly due to land and river-based anthropogenic nutrient inputs, with the evolution of massive agriculture and the use of fertilizers [1-3]. The seafloor in the Persian Gulf, as a shallow basin, is typified by ecologically and economically valuable benthic species. Low concentration of dissolved oxygen could lead to significant losses in biomass and diversity. Here, dissolved oxygen results of several research cruises to the Persian Gulf and the Strait of Hormuz during 2018-2019 on the research vessel Kavoshgar Khalij Fars were discussed. The results showed that summer to autumn hypoxia ($O_2 \leq 61$ µmol/kg) occurs mainly at depths ≥ 50 m to the bottom in the Persian Gulf. This seasonal hypoxia starts in late summer (when the strong stratification prevents ventilation of the water column) in the near-bottom layer reaching its greatest severity in mid-autumn with an unexpected maximum area of more than 50,000 km^2. The minimum oxygen measured at the near-bottom layer of the western basin in autumn (25.8 µmol/kg or 0.85 mg/l) was lower than any previous measurement in the open waters of the Persian Gulf. In the Strait of Hormuz, the seasonal hypoxia appears in early summer in the near bottom of the most eastern part at the Iranian side, which is less affected by the outflowing Persian Gulf Water. Although the highest hypoxic area in the Persian Gulf was observed in autumn, the greatest area and thickness of low-oxygen waters ($O_2 \leq 92$ µmol/kg) in the Persian Gulf occurred in late summer. Deepening vertical mixing in late autumn and destratification and full vertical mixing of the water column due to the surface cooling in winter are suggested as the foremost influential force of hypoxic dissipation. In the hypoxic and low-oxygen areas, high phosphate and nitrate concentrations and low pH values were found. pH values recorded in hypoxic waters were as low as what is predicted for surface ocean under ocean acidification in 2100 (assuming the worst-case CO_2 emissions scenario). Considering the significant hypoxic and more acidic waters of the bottom layer in the late summer and autumn, we strongly suggest evaluating the effects of hypoxia and acidification on the Persian Gulf ecosystems [4].

Keywords: Deoxygenation, acidification, Persian Gulf, Persian Gulf Explorer

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Synthesis of PAN/CZMA-LDH Electrospun Nanofibers as a New Sorbent in The Microextraction on Screw of Organophosphorus Pesticides from Vegetable Samples

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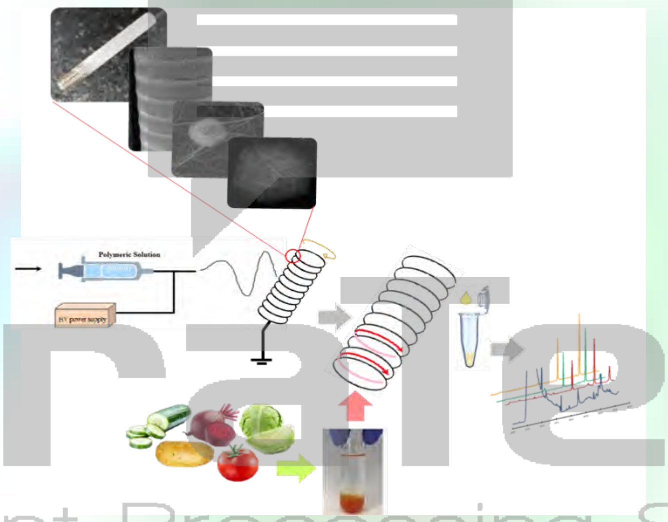
Graphical Abstract



Abstract: Organophosphorus pesticides (OPPs) are widely used to control the yield of agricultural products. But OPPs are highly toxic even at low concentrations, and can be transferred to human food chain through different ways. Therefore, the detection and determination of OPPs is fundamentally essential [1]. Due to the low concentration of OPPs in the real samples and the matrix complexity of the real samples, it is very challenging to measure OPPs accurately and precisely. Employing an extraction technique may be useful for overcoming the mentioned challenges. Solid-phase microextraction (SPME) is a class of the sample preparation methods with significant advantages, such as, the reduction or absence of organic solvents, and enhanced sensitivity due to concentration of analytes in a small extraction phase [2]. Microextraction on screw (MES) is one of the SPME techniques that is able to eliminate the disadvantages

of conventional methods, in this method a screw was utilized as a substrate and its surface was coated with the desired sorbent. Passing the sample solution through the spiral path of the grooves on the screw surface increases the contact surface between the sample solution and the sorbent, thus the extraction efficiency increases [3]. This research is an attempt to expand the recently reported MES method. For this purpose polyacrylonitrile/calcined ZnMgAl-LDH nanofiber was fabricated with the aid of the electrospinning technique on screw surface and applied for extraction of OPPs from agricultural samples. Separation and determination of OPPs was performed by GC-MS spectrometry analysis. Characterization of the fabricated nanofiber was carried out utilizing FTIR spectroscopy, FESEM and EDX. Effective parameters on extraction efficiency of the analytes including sample pH, ionic strength, sample flow rate and number of cycles, type, volume and flow rate of desorption solvent were optimized using one variable at a time method. Under the optimized conditions, the limit of detection were 0.03 and 0.07 μg L^{-1} for diazinon and chlorpyrifos, respectively. This method showed good linearity in the range of 0.10-1000.00 μg L^{-1} for diazinon and 0.25-1000.00 μg L^{-1} for chlorpyrifos with $R^2 > 0.996$. The intra- and inter-day precisions (RSD%, n = 3) were ≤ 6.4% and ≤ 7.7%, respectively. Also, RSD% values less than 11.1% were obtained for screw to screw reproducibility. To investigate the extraction efficiency, PAN/CZMA-LDH was employed to analyze various vegetable samples, including cabbage, potato, tomato, cucumber and beetroot where it led good recoveries ranged between 65% and 84%.

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Using Colorimetric Nano-sensor to Detection of Corona Virus

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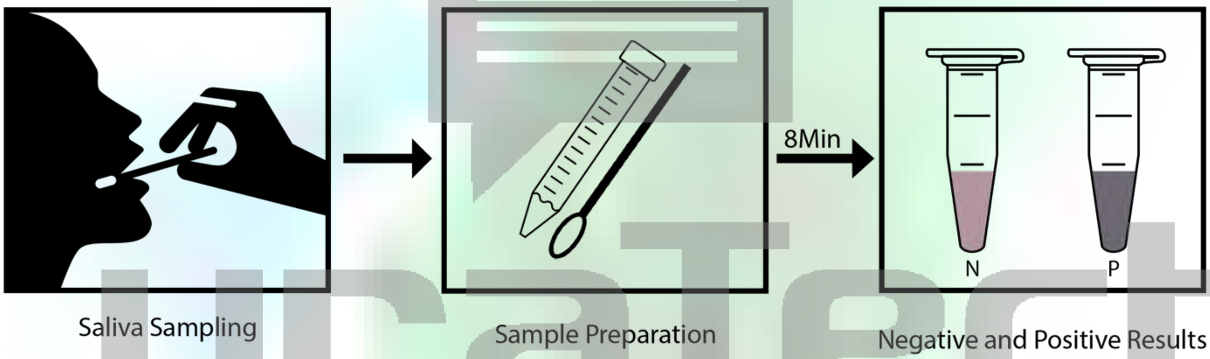
Graphical Abstract



Abstract: The new coronavirus (SARS-CoV-2) outbreak was recognized in December 2019 and it has caused the death of many people [1]. As of 5th August 2021, approximately 200 million COVID-19 confirmed cases worldwide have been reported, resulting in the death of 4.26 million people [2]. Due to the prevalence of the disease caused by this virus, it is necessary for rapid and efficient diagnostic methods to identifying coronavirus in humans. Currently, the only available way to diagnose SARS-CoV-2 is the Real Time - polymer chain reactions (RT-PCR) method, which can detect virus genetic material (RNA) in samples collected from the patient's oropharynx and nasopharynx, but it is considered a time-consuming, high cost, and expert manpower method. Over the past decades, nanomaterials, including nano-sensors, have always emerged as one of the most promising options for innovation in traditional analysis methods [3]. Nanomaterial such as

gold nanoparticles (AuNPs) and silver nanoparticles (AgNPs) have plasmon resonance properties which are giving new opportunities for colorimetric sensors [4]. In this study, a nano-sensor based on functioned gold nanoparticles nano-particles has been developed. This nano-kit provides the ability to detect SARS-Cov-2 through saliva sample in 5 to 8 minutes. Compared to existing methods such as RT-PCR, colorimetric assay by nano-kit has a faster detection time, lower cost, no need for an expert technician. In this method, after sampling the patient's saliva, an oral-soaked swab is placed in the virus culture medium. The Saliva sample is combined with the sensor and reagents, then in the presence of the virus, the color changes occur. The results of this procedure can be seen by the naked eye by changing the color from light red to dark purple.

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Evaluation of Carbon Nanotubes Performance in The Lead and Cadmium Adsorption from Refinery Wastewater: Process Modeling by RSM

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Abstract: Supply of safe drinking water is crucial to human life, and safe drinking water should not impose a significant risk to humans. Although few heavy metals are essential for human health, an excess amount of these metals can have negative effects. The heavy metals are released into the environment through natural process and anthropogenic activities. The industrial processes generate wastes, which are mostly discharged into the environment. Lead (Pb) and cadmium (Cd) are among the heavy metals in surface waters, which may lead to adverse effects such as bone and lungs cancer, chronic headaches, dizziness, chest pain, body weakness etc. Hence, it is necessary to remove such heavy metals from drinking water sources. The aim of present study was to determine the efficiency of multi-walled carbon nanotubes to remove lead and cadmium from refinery wastewater. Batch adsorption experiments were carried out by varying main operational parameters such as pH, initial concentrations of Pb and Cd, carbon nanotubes dosages, and contact time. Experimental design was applied to reduce the number of experiments, save time and cost, determine the main effects of independent variables on response, and determine optimum conditions. Experiments were designed by central composite design (CCD) based on response surface methodology (RSM) using Design Expert, version 11 software. Based on the results pH, initial concentrations of heavy metals, and adsorbent (carbon nanotubes) dosage had main role in adsorption process. The findings demonstrated that the highest adsorption of Pd and Cd from aqueous solution was achieved under optimal conditions (Pb/Cd initial concentration: 50 mg L-1, pH: 5,adsorbent dosage: 0.25 g L-1, and contact time: 75 min).

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Poster Presentation

Study of Inhibitory Effect of Three Amino Acids Cysteine, Arginine and Proline as Green Inhibitors on Corrosion of Lead Alloy

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Abstract: One of the most effective and important ways to prevent metals corrosion is to use inhibitors. These compounds prevent corrosion of the metal surface by creating an impermeable barrier. Unfortunately, many inhibitors in aquatic environments are harmful to health. To solve this problem, in this study, the inhibitory effects of the three amino acids cysteine, arginine and proline on lead alloy coroosion in sulfuric acid medium were used. Amino acids are non-toxic compounds, inexpensive and can be prepared with a purity of more than 99%. On the other hand, as we know, lead is one of the heavy elements that have adverse environmental effects and causes water and soil pollution, therefore it is necessary to study of its corrosion. In this study, electrochemical techniques including dynamic polarization and electrochemical impedance as well as non-electrochemical techniques including weight loss measurement and scanning electron microscopy have been used. The effects of temperature, sulfuric acid and amino acid concentrations on the behavior of inhibitors have been studied. Corrosion data including corrosion rate and corrosion potential are obtained from dynamic polarization curves. Charge transfer resistance has been calculated using electrochemical impedance method. Also, electron microscope images show that increasing the concentration of inhibitor has reduced the corrosion rate of the alloy surface. The inhibitory efficiency depends on the type of amino acid and its concentration. The inhibitory efficiency of more than 99% has been measured in the presence of cysteine with a concentration of 0.1 M in a solution of 1 M sulfuric acid.

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Application of Magnetic Iron Nanoparticles to Remove Nickel Ions from Water

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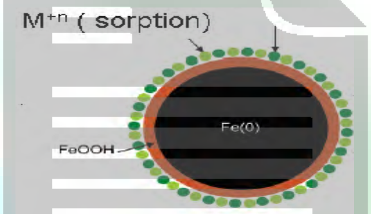
Graphical Abstract



Abstract: Magnetic iron nanoparticles are used as the core of new treatment systems to remove contaminants from groundwater and industrial wastewater. In this research, these nanoparticles have been used to remove nickel contaminants. For this purpose, experiments were designed and performed in two different ways. In the first method, the nickel-containing solutions were mixed with different amounts of iron nanopowder and then the solutions were irradiated with ultrasound. After certain periods of time, the magnetic particles were separated from the solution by magnetic field and their nickel residue was determined by atomic absorption spectrophotometer. The results show that iron nanoparticles have a high efficiency for removing nickel from water, so that using 0.03 g of iron nanoparticles, was removed about 13-25 ppm from nickel ion. Then, in the second stage, the separation process was performed using the osmosis phenomenon. In this stage, a system consisting of a solution of nickel in water and a nanofluid of iron in water separated by a semipermeable membrane, was designed. In this case, the conditions were adjusted so that the water in the nickel solution moved to the other side of the membrane due to its higher potential and thus separated from the nickel. Finally, with the help of magnetic properties, nanoparticles can be separated and pure water can be obtained.

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A Comparative Study of Modified and Raw Zeolite in Adsorption NH_4^+ from Wastewater

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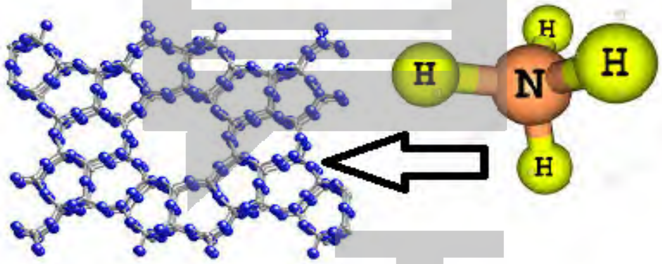
Graphical Abstract



Abstract: Various civilian, agricultural and industrial activities cause the presence of nitrogen compounds in surface and groundwater, where they are further converted into ammonia and its salts. The progressive increase in ammonium concentration in the environment represents a serious concern since it is one of the main causes of eutrophication and its transformation may lead to carcinogens. On the other hand, wastewater has recently been considered as a potential source of nitrogenous nutrients for plants, once adequate recovery processes have been provided. In this research used of modified and raw(unmodified) zeolite for adsorbtion Ammonium ions from wastewater. At first, the adsorbents transfer to nano sizes by mechanical method.Among the modified and raw adsorbents, the modified adsorbent showed better capacity adsorb in adsorbtion NH_4^+. Although NO_3^+ had high adsorbetion beside NH_4^+. The raw and modified samples were

characterized by XRD, FT-IR, SEM, BET and TG. The effects of analytical parameters such as pH of solution, particle size, sorbent weight, dose of ligand, concentration of NH_4^+ solution, pH of NH_4^+ solution, contact time, shaking rate, regeneration and selectivity were studied. The sorbent weight was determined 0.07g and such as, pH of solution of ligand was 5. The modified adsorbent prosses on zeolite depend on pH and other parameters. The important method in experimental adsorbtion of NH_4+ was ion exchange**.** Results suggest that modified adsorbent might be a potential material for ammonium and nitrate removal from water.

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Synthesis of Layered Double Hydroxide Nanostructures for Adsorption of Crystal Violet Dye from Aqueous Solutions

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Abstract: Crystal violet is one such and common type of dye extensively used by the paper and textile industry. It is also used as a biological stain and dermatological agent in human and veterinary medicine. Despite its wide use, crystal violet has been found to have harmful effects on humans and has been suspected to be a potential carcinogen. Consumption of the dye even in a small amount (< 1 ppm) may result in respiratory disorders, kidney failure and permanent blindness. Its exposure to large amounts irritates the skin and the digestive tract. Belonging to the class of triarylmethane dyes, it has a complex chemical structure and long half-life which results in their persistence in the environment for a very long time, aggravating the problem further. The dye has also been found to be teratogenic and mutagenic and is thus, categorized under biohazards. Therefore, it is necessary to focus more on removing such dyes from industrial wastewater before reusing or discharging them into the aquatic environment. Layered double hydroxides (LDHs) contain hydrocarbons and hydrotalcite-like compounds that have high adsorption efficiencies. these compounds have positive properties such as greater area, high thermal stability, stability over a wide pH range, greater adsorption and recyclability, and therefore absorption of pollutants are suitable compounds of water. Here, LDH Ca-Al-SDS are prepared by simple chemical methods and then contaminated water is used to absorb the crystal violet dye. In addition, the results showed that the synthesized LDH effectively removed the crystal violet dye up to 95% and can be used in wastewater treatment to remove cationic dyes very efficiently.

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Preparation and Study of Photocatalytic Activity of Graphitic Carbon Nitride for The Removal of Pharmaceutical Pollutants

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Abstract: Excessive consumption of drugs, as well as wastes from the pharmaceutical industry and hospitals, has increased the concentration of these pollutants in the aquatic environment and even drinking water. These chemicals pose a major danger to human and environmental health due to their degradable nature, even in small quantities. Therefore, the effort to remove them from the water sources is essential. In this regard, graphitic carbon nitride via a cost-efficient method was prepared using thermal polymerization of urea. Its photocatalytic activity was studied for the removal of pharmaceutical pollutants ibuprofen and ofloxacin. The results of the experiments show that the produced graphitic carbon nitride can remove 73% and 33% of ofloxacin and ibuprofen from the aqueous medium**,** respectively.

Keywords: Graphitic carbon nitride, Photocatalyst, Pollutant, Pharmaceutical, Ofloxacin, Ibuprofen

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Geochemistry of Arsenic (As) In the Surface Sediments of Qaen, Iran

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Abstract: Arsenic occurs naturally in the earth's crust and is widely distributed in the environment. WHO has set the permissible limit of arsenic in drinking water at 10 μg/l and various literatures have reported this limit for the soil to be 20 mg/kg.This paper attempts to document the concentration of arsenic and in sediments of the 1:100,000 scale Qaen quadrangle map. Sediment samples indicate content of as which ranges from 6.9 to 53.2 mg/kgwith a mean concentration of 11.9 mg/kg. The geoaccumulationindex (Igeo) results showed that the as levels ranged from uncontaminated (Igeo< 0) to polluted. The results from this study can helpprevent potential cumulative risk and improve the implementation of effective environmental risk controls at large-scale as contaminated sites.

Keywords: Arsenic, geoaccumulationindex (Igeo),WHO, Qaen.

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Mango Peel Activated Carbon Functionalization with Acid Anthranilic for Efficient Removal of Uranium from Radioactive Effluents

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Abstract: As a toxic and radioactive metal, uranyl ions have a high potential for human health and environment. It is known that it causes organ failure and death due to accumulation in organs with radioactive properties and various compounds formed in metabolism even at very low concentration in environmental drinking water [1]. The predominant form of uranium species in the aqueous medium is hexavalent uranyl ion, which is leaked from natural sources and artificial plants. There are many physicochemical methods including precipitation, filtration, biological treatment, and adsorption for recovery of this ion from environment and wastewater [2]. Among the techniques, adsorption method outshined good advantages such as easy usability, cheap method, and reusable adsorbent design. The purpose of this study was modification of activated carbon (AC) to prepare a new selective sorbent for removal of uranium ion. The modification was performed by introducing carboxyl groups onto AC using APS solution followed by functionalization with acid anthranilic (AA) as a selective ligand for U(VI) ion (UO_2^{2+}) adsorption. The characterization of the synthetized sorbent (AC-AA) was accomplished by several methods including potentiometry, SEM, EDS, XRD and FT-IR to confirm successful functionalization of the sorbent surface with oxygen and amine groups. The sorption of U(VI) on the unmodified AC and AC-AA was investigated as a function of contact time, sorbent content, initial uranium concentration, solution pH, and temperature using batch sorption technique. In addition, the effect of various parameters on the U(VI) sorption capacity was optimized by the response surface methodology as a potent experimental design method. The results indicated that sorption of U(VI) under the optimal conditions was significantly improved onto AC-AA compared to AC. Kinetic studies displayed that the sorption process reached equilibrium after 100 min and followed the pseudo-second-order rate equation. The isothermal data fitted better with the Langmuir than the Freundlich model. The maximum sorption capacity of AC-AA for U(VI) was obtained to be 192.3 mg g^{-1} by the Langmuir model under optimum conditions, which demonstrates the sorption capacity has been improved by the modification process. The thermodynamic parameters (ΔH, ΔS and ΔG) indicated that sorption of uranium onto AC-AA was an endothermic and spontaneous process. The sorption studies on radioactive effluents of the nuclear fuel plant represented high selectivity of AC-AA for removal of uranium in the presence of other metal ions, and the selectivity coefficients significantly improved after modification of the sorbent. Application of AC-AA for treatment of industrial effluents containing heavy and radioactive metal ions show high potential and capability of the proposed method.

Keywords: Uranium recovery, Mango peel, Activated carbon; acid Anthranilic,Waste Treatment

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Statistical Optimization of Hollow Fiber Liquid Phase Microextraction for Preconcentration and Determination of Strychnine

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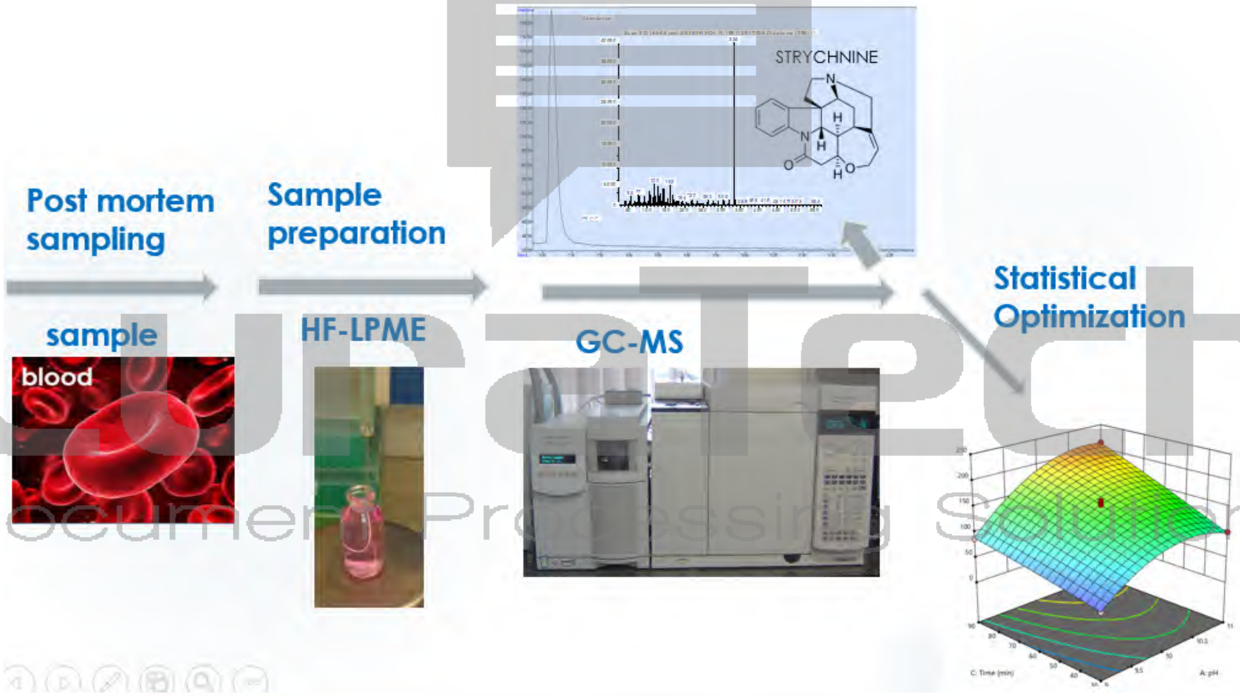
Graphical Abstract



Abstract: A sensitive and reliable extraction method based on the two-phase hollow fiber liquid phase microextraction followed by gas chromatography–mass spectrometry has been developed for determination of strychnineas an extremely poisonous alkaloid.Strychnine is obtained from Nux Vomicaand its fatal dose is in the range of 30–90 mg [1,2].A Box Behnken design (BBD) with three variables including the extraction time (30, 60, 90 min), pH (9, 10, 11) and ionic strength

(1, 2, 3 mol L-1) was used to optimize the extraction process. The results were satisfactorily fitted to a quadratic response surface model with R2=0.9792 and F=34.36 which predicted the optimum conditions of operation (extraction time of 89 min, pH=11 and ionic strength of 3). Based on the results,the ionic strength, extraction time and pH had significant effects on the extraction process. The method detection limit and limit of quantitation were obtained as 5 and10 µgL-1, respectively. The calibration curve was linear in the range of 10-1000 µg L-1 with a correlation coefficient of 0.9947. The results suggested the proposed methodas an environmentally friendly analytical methodwith a total consumption of40 µL of the organic solvent for each extraction, for highly efficient preconcentration and trace determination of strychnine in the biological fluids and environmental aqueous samples.

Keywords: Hollow fiber liquid phase microextraction, Gas chromatography-mass spectrometry, Strychnine, Response surface methodology, Box Benken design

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Removal of Methyl Orange Dye Using Polyaniline Modified Walnut Shell

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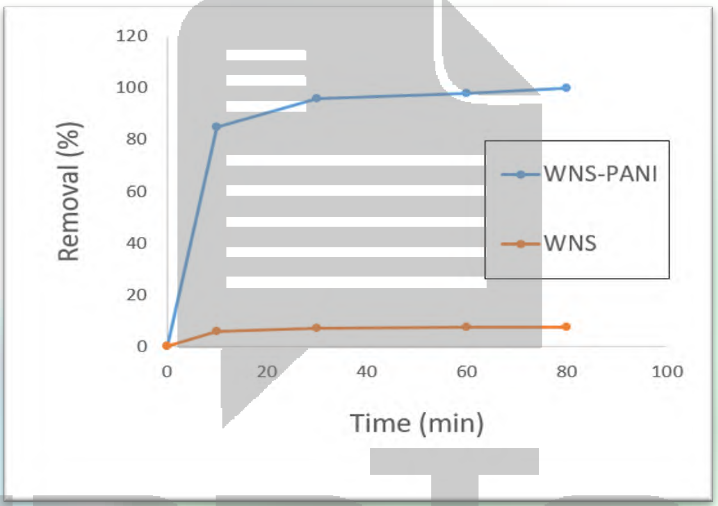
Graphical Abstract



Abstract: Exposure to water pollutants is one of the major threats to human health. Annually, large volumes of wastewater enter the environment from industrial, agricultural and domestic units, including high concentrations of organic and inorganic chemicals such as hydrocarbons, dyes, Pesticides and heavy metals [1].There are several common methods for minimizing these harmful pollutants. Among these methods, the adsorption process by low-cost and simple operation biosorbents coated by polymers with porous structuresis a good option for removing pollutants from water[2].

In this study, polyaniline-modified walnut shell used as sorbent to investigate the removal of methyl orange dye from water. The polyaniline-modified walnut shell was prepared by in-situ polymerization of aniline in the presence of walnut shell powder. After polymerization, the produt was washed with distilled water and then dried in an oven at 60 centigrade degree. The sorbent was characterized by field emission scanning electron microscopy and FT-IR spectroscopy. Removal experiments were performed at room temperature and pH= 4.5, with dye initial concentration of 25 mg/L over 80 minutes. Dye concentration was determined at time

intervalsbymeasuring the absorption values using UV-vis spectrophotomrty at λ_{max} of 464 nm. As can be seen in the figure above, unmodified walnut shell is not able to remove the dye. while after modification with polyaniline, the removal efficiency and capacity reach 100% and 125 mg/g (in 80 minutes), respectively. These results show that modifying walnut shell with polyaniline has a significant effect on removing methyl orange dye.

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Polyaniline Emeraldine Salt for Removal of Dyes from Wastewater

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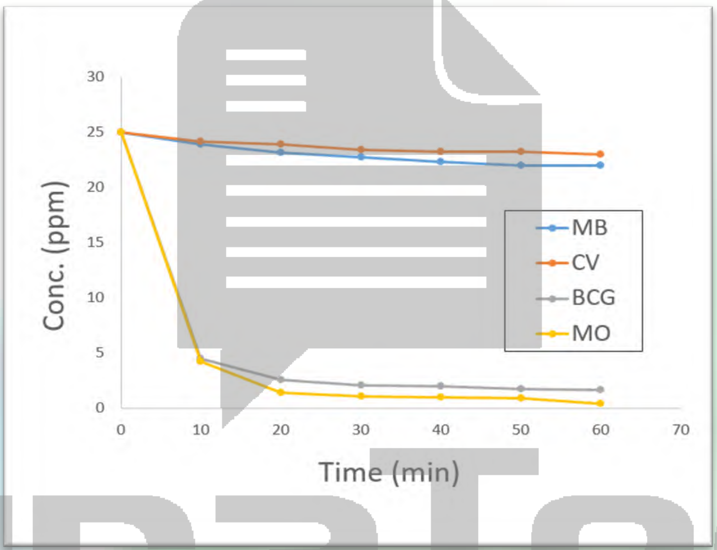
Graphical Abstract



Abstract: Water pollution is one of the recent concerns of the whole world. Because A large number of natural and unnatural pollutants have been released from human and industrial resources and have rapidly reduced the quality of water resources. These pollutants have many destructive effects that can be a major threat to human health. Therefore, the removal of water pollutants is very important [1]. There are several common methods to minimize these pollutants, such as filtration, precipitation, coagulation and adsorption. Polymeric materials possesingthe active sites such as polyaniline have been investigated for the removal of aqueous contaminants [2].

In this study, nano fibers of polyaniline synthesized in the emeraldine salt (ES) form and used as adsorbent to investigate the removal of several different cationic and anionic pollutants from aqueous media. Removal experiments were performed at room temperature and pH=4, with dye

initial concentration of 25 mg/L over 1 hour. The concentrations of pollutants were calculated according the Beer-Lambert law and by UV-vis spectroscopy at λ_{max} values of 464, 664, 424 and 591 nm for methyl orange (MO), methylene blue (MB), bromocresol green (BCG) and crystal violet (CV), respectively. The concentration of dye in the solution was monitored with time during the adsorption experiment. According to the results shown in the figure above, the emeraldine salt of polyaniline is not able to remove cationic dyes while it is an effective and selective adsorbent for the removal of anionic dyes. The removal of anionic dyes from water can be explained by electrostatic interaction between anionic concomitants and positively charged sites on the polyaniline emeraldine salt.

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Removal of Toxic Hexavalent Chromium from Aqueous Solutions Using Polyaniline Modified Pine Cone

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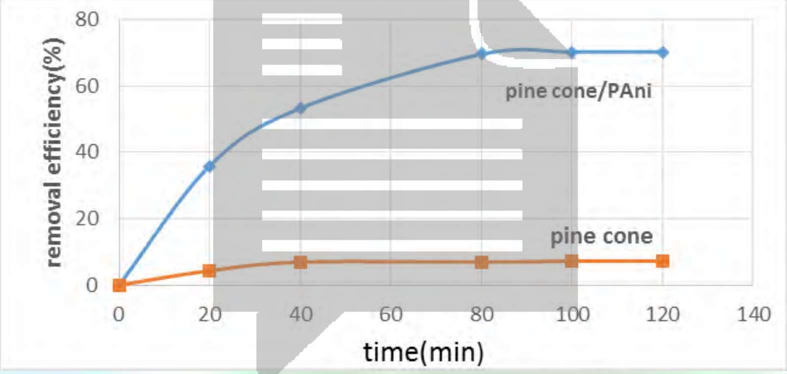
Graphical Abstract



Abstract: Growing industrial development and population explosion in the world resulted in an increasing amount of different pollutants daily discharged into the environment. Some pollutants, such as heavy metals, even at low concentrations, are harmful to human health. Chromium is not naturally found in water; however, it enters the environment as chromate and dichromate through industrial pollution[1]caused by effluents from metal plating, tanning, dye making, and stereotyping workshops and by oil varnish and ink. Several methods are used to minimize these harmful pollutants. The adsorption process using polymer modified biosorbents is a good option for removing pollutants from water due to low-cost and simple operation. In This work pine cone/polyaniline composite was prepared byin-situ polymerization of aniline in the presence of pine cone powder. After polymerization, the pine cone/polyaniline composite was washed with distilled water and then dried in an oven at 60 centigrade degree. Thepine cone/polyaniline composite was characterized by FT-IR spectroscopy. The composite was used as adsorbent to remove Cr (VI). As seen in the figure, modification of pine cone powder with polyaniline intensively enhanced the chromate removal. The removal of chromium from water can be

explained by electrostatic interaction between negatively charged chromate and positively charged sites on the polyaniline emeraldine salt. The removal efficiency was reached over 70 percent after 80 minutes. The equilibrium adsorption capacity increased from 8.9 mg/g for pine cone powder, to 78.2 mg/gfor pine cone/polyaniline composite as a result of modification of pine cone powder with polyaniline.

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Kinetic Study of Photocatalytic Degradation of Solochrome Black T in Aquatic System Using Semiconductor Oxides in Various pH

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Abstract: Photocatalytic treatment of pollutants in aquatic environments is an active research area in recent decades. Marine and fresh waters are mixtures of dissolved inorganic and organic compounds, biological species and colloidal aggregates. Photocatalytic degradation by semiconductors as photocatalysts is regarded to be an efficient means of treatment for dyes owing to its incomparable superiority, being ecologically friendly, highly efficient and with good stability [1-3]. The use of semiconductor materials, as a means for degrading the pollutants present in the environment under UV light has been broadly investigated in the last few years. Among semiconductors titanium dioxide is one of the most popular and promising materials as a photocatalyst [4-7]. Solochrome Black T; is toxic for eye, skin and also is respiratory irritant. Therefor degradation study of it seems to be in demand for environmentally chemistry point of view.

In continuation of our ongoing programme in wastewater treatment, in this research, photocatalytic degradation of aqueous solution of Solochrome Black T; was carried out over TiO2 (anatase and rutile) in a photoreactor. The observed results revealed that the order of photocatalytic activity for degradation of selected compounds was TiO2 (anatase)> TiO2 (rutile). The effect of some physical and chemical parameters such as amount of photocatalyst, pH, time of irradiation and solvent were studied. The photodegradation of the dye obeyed a pseudo-first order kinetics according to the Langmuir-Hinshelwood model at all used buffer pH. The observed rate constants (k(obs), the Langmuir-Hinshelwood rate constants, k(r), and adsorption constants, KA are reported for current process at various buffer pH.

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Potential Risk of Mercury to Human Health in Muscle Tissues of Sander luciopercan from South Caspian Sea

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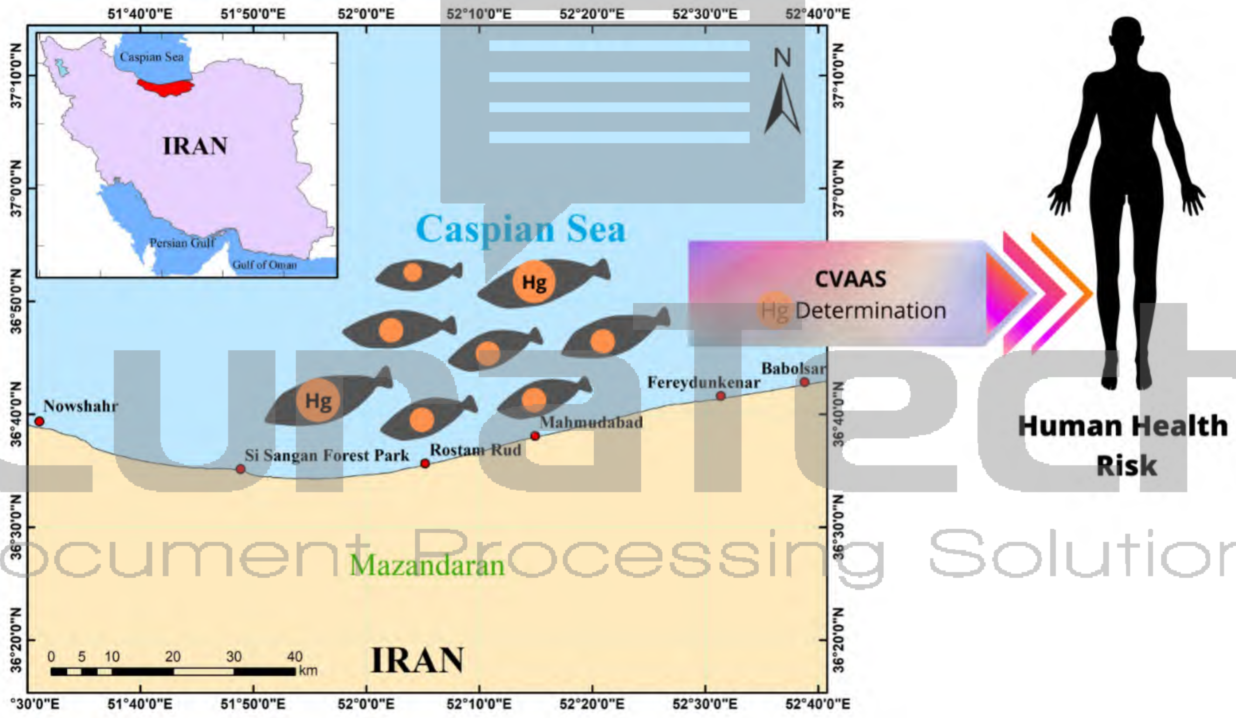
Graphical Abstract



Abstract: Fish is considered to be an important source of high quality proteins and other nutrients (long chain polyunsaturated fatty acids, particularly omega-3 and omega-6 fatty acids, vitamins and trace elements) for people all over the world (1-4). Many health advantages have been documented of regular fish consumption, such as reducing risk of cardiovascular diseases and

improved neurodevelopment (5, 6). Therefore, recently, per capita fish consumption has increased and Sea products play a considerable role in the food supply for people all over the world (7). However, Sea products may also be contaminated by chemical contaminants, such as heavy metals. Since aquatic ecosystems receive a large amount of heavy metals, fish and other aquatic organisms are the main organisms to be affected by pollutants (8). When the metals are released into aquatic environments, particles can absorb them via biogeochemical cycles which can caused to lethal or sub-lethal effects on the ecosystem (9, 10). With respect to the importance of the issue mention above and its dangers and complications, so many researchers have investigated the heavy metals in marine ecosystems all over the world (11-18).The Caspian Sea is the largest lake in world, with an area of 378400 km2 and a basin volume of 78170 km3, respectively (19). It islying between Europe and Asia and surrounded by five countries—Iran, Kazakhstan, Turkmenistan, Azerbaijan, and Russia (20). This study was conducted to determine the concentrations of Mercury (Hg) in the muscle tissues of Sander lucioperca and collected from Mazandaran, the Caspian Sea, Iran. Additionally, risk assessment of consumers to exposure to metals through fish consumption was estimated. Mercury has been measured by using Cold Vapor-Atomic Absorption Spectrophotometry. The mean concentration ± standard error was calculated to be 0.40 ± 0.03 (µgg-1 dry weight) for the heavy element Mercury of Sander lucioperca's muscle tissues.

The hazard quotient values showed that consumption of the analyzed fish posed a health risk to consumers in some stations. The fishes contamination of some of the examined stations such as Nowshar station exceeded acceptable limits according to FAO, WHO, FDA, and EC indexes.

Given the importance of these ecosystems to people around the world, we need to monitor and evaluate these areas every year.

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Ion mobility Spectrometry for Evaluation of Iron Oxide Magnetic Nanoparticles Ability to Adsorb Nalidixic Acid

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Abstract: The contamination of water by organic pollutants, especially pharmaceutical contaminants, is one of the concerns all over the world. Among the various water pollutants, antibiotics are of particular interest to researchers because of the risk of increasing antibiotic resistance. Nalidixic acid (NA) is the first commercialized antibacterial quinolone [1].Ion mobility spectroscopy (IMS) is a separation method that works at atmospheric pressure. The advantages of ion mobility spectrometer are high sensitivity, low detection limit, simple operation and low cost [2]. In the present study, ion mobility spectrometer was used to measure nalidixic acid residues in aqueous solution. The removal of nalidixic acid from water by adsorption on iron oxide magnetic (Fe_3O_4) nanoparticles has been investigated. In order to do this, Effect of NA initial concentrations (30-80ppm), effects of pH (2-12), and contact time (0.5,1-5hours)in removing of NA from aqueous solutions were investigated**.** Transmission electron microscope (TEM), and FT-IR were used to identify the characterization of synthesized Fe_3O_4 nanoparticles**.**

The results indicated that 87.6 % of the NA concentration removed by Fe_3O_4 in the optimal conditions including pH=12, temperature25 °C, NA concentration 80 mg/L, contact time 5 hours and adsorbent dose 0.5mg/L. The resulting data from adsorption experiments had better correlation with the Freundlich isotherm and *pseudo*-second order kinetic model. The results of this study demonstrate that iron oxide magnetic (Fe_3O_4) nanoparticles is a suitable adsorbent for antibiotic removal from aqueous solutions.

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Ultrasound Enhanced Activity of Ozone for Degradation of Catechol in Aqueous Solution

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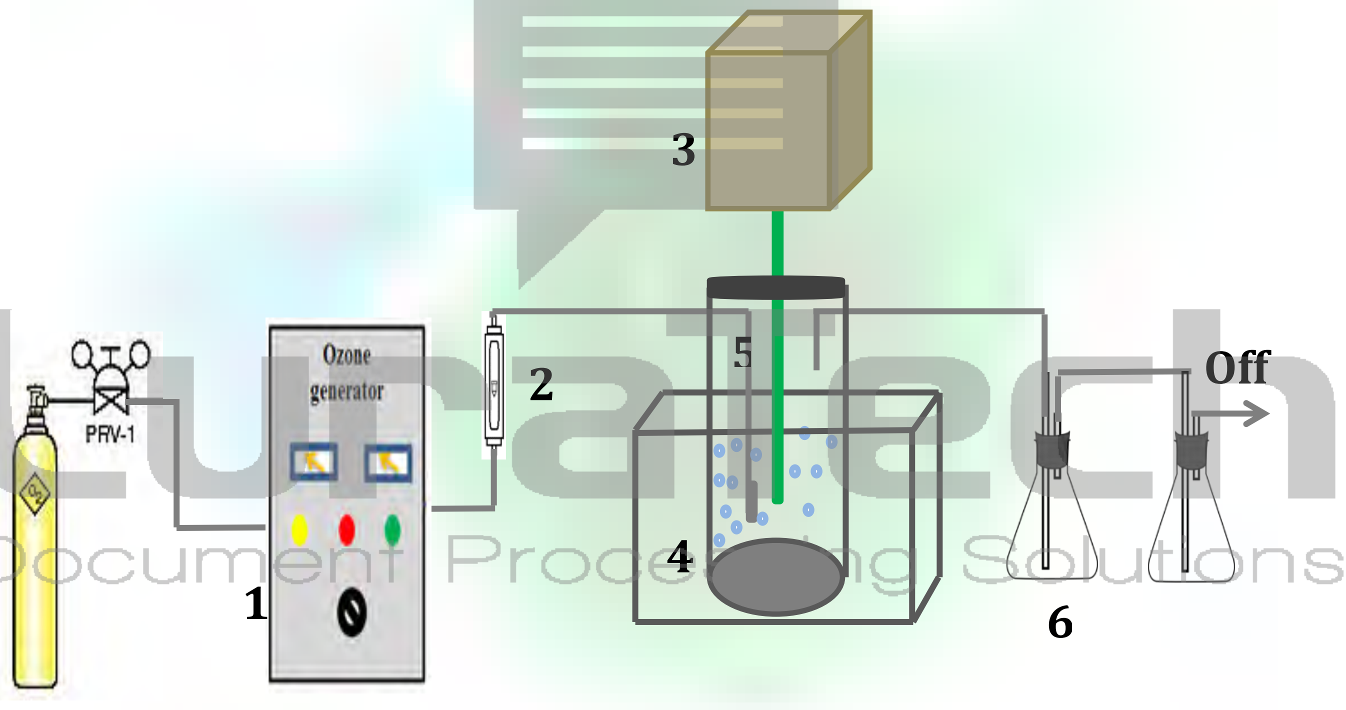
Graphical Abstract



The experimental set-up: (1) ozone generator; (2) rotameter; (3) temperature controlled bath; (4) ultrasonic generator; (5) reactor (6) absorption bottle.

Abstract: Nowadays, water pollution caused by diverse poisonous compounds, particularly hydroxy aromatic compounds and their derivatives, has become a prominent environmental issue because of the possible toxicity to human beings. Advanced Oxidation Processes (AOPs) have been developed as an emerging technology for treating hazardous organics in wastewater and groundwater. The degradation and mineralization of Catechol in aqueous solution was investigated by various advanced oxidation processes including US, O_3 and US/O_3. The obtained results revealed that the coupled US/O_3 process is the most effective method for this purpose. Then, the effect of operational parameters, such as ozone dosage, US power and pH on the degradation and mineralization of pollutant on coupled process was studied. The results demonstrated that the ozone dosage and US power were found to have the noticeable impact on the process; however, initial pH was less effective. Optimum condition of US/O_3 process is ozone concentration of 5.2 mg/L, Us power of 0.4 W/mL, pH = 6.5, Catechol concentration = 50 ppm and reaction time = 20 min. According to experiments, the percentage of Catechol removal in this condition was 99.8Finally, degradation intermediates were identified by the GC-MS method (Maleic acid, Oxalic acid) under optimized conditions.

Keywords: Degradation; Mineralization; Ultrasound; ozonation;Catechol; US/O_3

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Electrochemical Detection of Hydroquinone Using Electrochemical Sensor Based on Ionic Liquid and Nano-Composite

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Abstract: Hydroquinone is an isomer of phenolic compounds, which is considered as environmental pollutants by the US Environmental Protection Agency (EPA) and the European Union (EU) [1]. It is also present in cosmetic formulations of products for coating finger nails and hair dyes, tanning, pesticides, flavoring agents, medicines, and photography chemicals [2] and can easily be introduced into the environment as pollutants. Recent pieces of evidence showed that hydroquinone is able to enhance carcinogenic risk by generating DNA damage and also to compromise the general immune responses which may contribute to the impaired triggering of the host immune reaction. Therefore, detection of Hydroquinone in various samples is very important.as yet many methods have been established for the determination of Hydroquinone, including high-performance liquid chromatography [3,4], synchronous fluorescence [5], spectrophotometry [6,7], electrochemiluminescence [8] and electrochemical method [9]. Among them, electrochemical methods are preferable, and attractive due to the advantages of fast response, low cost, high sensitivity and selectivity. 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. 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. The electrochemical-based sensors showed more advantages in recent years dueto fast analysis, wide diversity and low cost.In this work, an electrochemical sensor for detection of Hydroquinone and catechol was developed based on the CuO/N-doped reduced graphene oxide nano-composite and IL modified carbon paste electrode (CuO/N-rGO/CPE). Compared with unmodified CPE, the CuO/N-rGO/CPE exhibited excellent electrochemical activity for the determination of Hydroquinone. The experimental results showed the wide linearity range, with lower limit of detection for determination of Hydroquinone

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Environmental Geochemistry of Toxic Heavy Metals in Surface Sediments of Qaen, Iran

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Abstract: Heavy metals are naturally present in our environment are dangerous for the due to their toxic and stable behavior in nature. In this study, to evaluate the risk of heavy metals pollution, a dataset of stream sediment elemental concentration of the 1:100,000 scale Qaen quadrangle map was used. The mean concentrations of Cu, Pb, Zn, Cr, Co, and Ni in the surface sediments of the study area were 21 mg/kg, 22 mg/kg, 57 mg/kg, 62 mg/kg, 12 mg/kg and 40 mg/kg, respectively. The methods forcalculation of pollution indices such as Enrichment Factor (EF), Contamination Degree (CD) and Contamination factor (CF) are considered to know the level of heavy metal pollution in the study area. The results of pollution indices suggest that almost all the sites are polluted by heavy metals. The data could be very useful to metal pollutants and their sources in the surface sediments.

Keywords: Heavy metals, Enrichment Factor (EF), Contamination Degree (CD), Contamination factor (CF), Qaen.

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Heavy Metalremovalby Using Magnetic Nanoparticles Loaded onto Activated Carbon

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Abstract: Heavy metal ions such as copper، iron، nickel، leadetc in the environment are of major concern due to their toxicity to many life forms. Unlike organic pollutants، which are susceptible to biological degradation، metal ions do not degrade into any harmless end products [1] and tend to accumulate in living organisms، causing various diseases and disorders [2]. Heavy metal contamination exists in aqueous waste streams of many industries، such as metal plating facilities، mining operation and tanneries. Therefore، elimination of heavy metals from water and wastewater is very important. The most widely used methods for removing heavy metals from wastewater include ion exchange، chemical precipitation، reverse osmosis، evaporation، and membrane filtration and adsorption [3]. Most of these methods suffer from some drawbacks such as high capital, operation cost and the disposal of the residual metal sludge which are not suitable for small-scale industries. Among various techniques، the adsorption process used exclusively in water treatment and many studies have been carried out to find inexpensive and chemico-physically feasible adsorbent [3]. Many reports have appeared on the development of low cost activated carbon from cheaper and readily available materials [4]. Activated carbons with their high surface area، micro porous character and chemical nature of their surface have made them potential adsorbents for the removal of heavy metals from industrial wastewater. In the present study, magnetic activated carbon was used to removal of heavy metals. The removal of heavy metals from aqueous solutions with magnetic activated carbon was studied by varying the parameters such as pH, the amount of adsorbent, initial concentration, adsorption time and temperature. Analyses of heavy metals (iron, copper and lead) in the samples were down by using flame atomic absorption spectrometer (FAAS). The maximum removal percentage of Fe^{+2},Pb^{+2} and Cu^{+2} was achieved at an adsorbent loading weight of 0.1 gr/L at pH=7 after30 min. Results showed that magnetic adsorbents could be re-used for 7 cycles.

Keywords: Magnetic adsorbent; Heavy metals; Removal.

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Preparation of Novel Electrospun Nanofibers for Extraction Two Herbisides (Atrazine and Ametrin) and Determination of Trace Amount of Them with Ionic Mobility Spectrometer (IMS) in Various Real Samples

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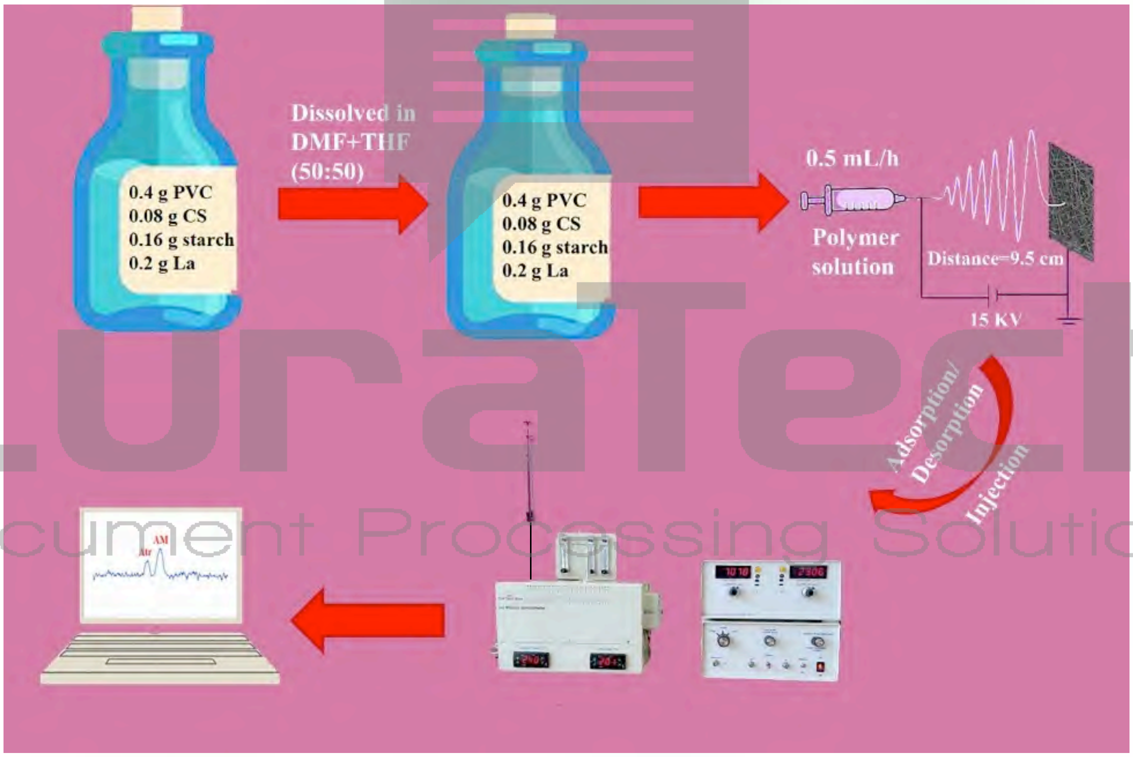
Graphical Abstract



Abstract: Atrazine (AT), 2-chloro-4-(ethylamine)-6(isopropylamine)-s-triazine and Ametrine (AMT), (N2-ethyl-N4-isopropyl-6-methylthio-1,3,5-triazine-2,4-diamine) are herbicides which have been used widely sofar **[1]** . Due to their effect on human health and environment, their

determination in real samples such as water, vegetables, and milk are essential **[2,3]**. To decrease matrix effect, sample preparation is necessary. Sorbents play significant role in sample preparation methods. Electrospun nanofibers with prominent features like large specific surface area and high prosity are excellent candidate as sorbents. Here, the electrospun composite of poly vinyl chloride/ethylene vinyl acetate/chitosan/starch (PVC/EVA/CS/Str) was prepared and used as promising in micro solid phase extraction of AT and AMT prior to CD-IMS analysis. From the evaluation of FE-SEM, FT-IR, XRD and TGA, the synthesize of electrospun nanofiberswas confirmed. Effective factors on adsorption and desorption steps optimized with Design-Expert 12.0 software. under the optimize conditions, the calibration plots were linear in the range 0.008-0.3 ppm. Limits of detection of $1.68*10^{-5}$ ppm and $4.6*10^{-6}$ ppm were obtained for AT and AMT, respectively.

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Bacterial Strains from Tannary Waste Polluted Soil Showed Heavy Metal Resistance and Bioaccumulation Capacity

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Abstract: Tanning is the process of treating skins and hides of animals to produce leather. Various chemicals are being used in this process and accordingly, tannery wastewater contains the variety of toxic heavy metals like chromium, cadmium, cobalt, lead, nickel, selenium and arsenic (1). Hence these regions are suitable sources for obtaining heavy metal resistance bacteria with application in bioremediation. In this study we isolated the bacterial strains from tannery effluent polluted soil and evaluatedtheir resistance to some heavy metals and their potentials for application in bioremediation process. The desired dilutions of soils were inoculated in the nutrient agar media containing 50 ppm of each arsenic, chromium, copper, lead and zinc ions. A total of 12 strains were obtained where their tolerances to heavy metals for the arsenic, chromium, copper, lead and zinc were as 2000 ppm, 2900 ppm, 1600 ppm, 3300 ppm, and 1600 ppm, respectively. In order to identify the bioaccumulation capacity of these strains, bacterial suspensions were inoculated in the 100ml Erlenmeyer flasks containing nutrient broth that supplemented by 50 ppm of each mentioned metals. The cultures were kept at 30 °C and agitation at 150 rpm for 72 hours. Bacterial cell pellets were removed by centrifugation (1000 g for 10 min) and the supernatants were passed through 0.45 µm filters. The potentials of bacterial strains to accumulate metals were determined based on the measurements of the remaining amount of primary metals in the supernatant by the inductively coupled plasma optical emission spectrometry (ICP-OES) (SPECTRO ARCOS, Germany) (2). The highest remediation rates for arsenic, chromium, copper, lead and zinc were as 6.7% (strain TP4), 13.1% (strain TN3), 9.9% (strain TP4), 76.9% (strain TN3), and 1.2% (strain

TN3), respectively. The results of this study showed that tannery waste contaminated soils are good candidates to obtain of bacterial strains with the potentials in bioremediation.

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Green and Environmentally Friendly Synthesis of Zinc-Based Metal-Organic Framework, Its Characterization and Analysis

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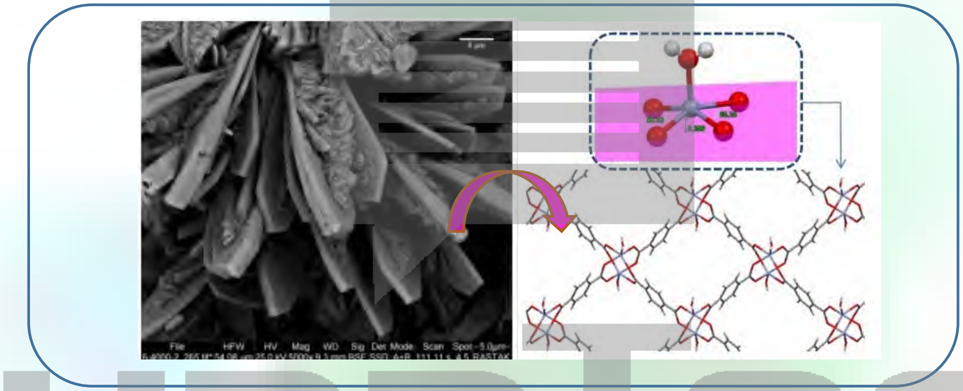
Graphical Abstract



Abstract: Ultrasound as green process and an alternative energy source was investigated for the environmentally benign synthesis with short reaction times, good selectivity and high yields reported [1,2]. One of the pioneering and interesting metal-organic framework material, called MOF-2 and having the formula [$Zn_2(BDC)_2$] [3]. Here we report an alternative approach to the synthesis of nanosheet structure zinc-based metal-organic framework that it was developed by treating zinc ions and terephthalic acid with ultrasound irradiation at room temperature.MOF-2 has been characterized by elemental analysis, FT-IR, Mass spectroscopy, powder X-ray diffraction (PXRD) and thermogravimetric analysis(TGA), all of the results supporting the good quality of the material. Surface morphology, shape and size of prepared compound was observed by scanning electron microscopy (SEM). The nanoporous nature of the prepared MOF-2 was verified by N_2 adsorption/desorption result.

Keywords: Ultrasound, metal-organic framework, nanosheet

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Synthesis of Modified Layered Double Hydroxide AsAn Efficient Adsorbent for Antibiotics Removal

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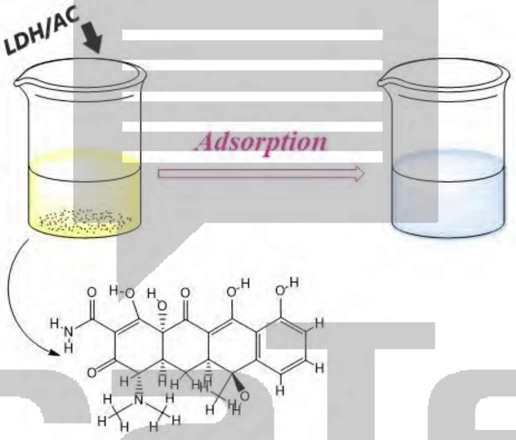
Graphical Abstract



Abstract: Water pollution and pollutants are an important issue and a major concern all over the world. Different pollutions have posed great dangers to the human communities and the ecosystem health[1,2].Layered double hydroxides (LDHs) are two-dimensional layered anionic clays That have received much attention due to their excellent physical and chemical properties. Their public formula is $[M_{1-x}^{2+}M_x^{3+}(OH)_2]$ $(A^{n-})_{x/n}$-mH_2O;M^{2+}, $M^{3+}$and A^{n-} demonstrate divalent and trivalent cations, and the interlayer anion respectively[3,4].The important properties of LDHs that leading to their abundant applications in the field of adsorption are: 1) their structural resistance to water, 2) their significant porosity and big space between layers, and 3) the presence of a large number of replaceable anions between the positively charged layers[5].Activated carbon (AC) is one of the known adsorbents for different types of contamination due to its porous structure and large surface area[6]. The combination of carbon nanomaterials (e.g., graphene, carbon dot, activated carbon, etc.) and layered double hydroxides leads to the creation of efficient nanocomposites with excellent properties as many properties of these two substances can complement each other[7].In this study, MgAl LDH/activated carbon (LDH/AC) nanocomposite as an eco-friendly adsorbent was synthesized successfully through a co-precipitation method and used for the removal of tetracycline (TC) antibiotics from aqueous solutions. The materials were characterized byX-ray diffraction (XRD) and FTIR spectroscopy. The effect of different parameters on the sorption process such as pH, adsorbent dose, contacting time, and initial concentration of TC was investigated. Central composite design (CCD) under response surface methodology (RSM) was utilized to determine the optimal conditions for TC antibiotic removal. Also, a statistically adequate model based on CCD was obtained to describe the effect of the variables on each other and operating variables on the sorption process. The optimum conditions of removal of TC antibiotic were pH=5.1, adsorbent amount: 0.11 g, initial antibiotic concentration: 50 mg/L, and contact time: 90 min. Under optimal conditions, about 91% of tetracycline was removed via LDH/AC adsorbent. Compared with the LDH and activated carbon pure, the as-prepared adsorbent showed a better performance towards the elimination of tetracycline.

Keywords: layered double hydroxide, Activated carbon, Tetracycline, Central composite design

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Green and Novel Synthesis of Heterocylic Compounds and Study Their Physicochemical Properties

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Graphical Abstract

Abstract: Green chemistry has been universally studied for many years. From the environmental and economic viewpoints, it is advisable to keep away from the utilization of dangerous and costly organic solvents. The utilization of water as the solvent shows valuable gains because it is very polar and thus immiscible with a majority of organic compounds [1]. Xanthene shows a number of biological activities such as antibacterial, antiviral, also their pH sensitivefluorescent property in laser technology. Hence, synthesisof xanthene derivatives are of a huge importance in biologicaland pharmacological studies [2, 3].In this research, due to the importance development of green chemistry, we wish to report green synthesis of novel, low cost, environmentall friendly with high reusability nanocatalyst using clinoptilolite, and study catalytic activity of it for green synthesis of xanthendion derivatives in water as solvent. The physicochemical properties of products studied and confirmed biological activity of xanthendion products.

Keywords: Nano, Green, Catalyst, Novel, Water, Xanten Dion.

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Nanotechnology and Plant Diseases Management

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Abstract: Every year, 20%–40% of harvests are lost because of plant diseases, resulting in billions of dollars of losses to crops agriculture. Although disease management options exist for many crops, all options possess significant shortcomings. This, taken with the building pressure for increased food production and the potential challenges caused by a warming climate, highlights the need for novel disease management approaches. Application of nanotechnological in plant diseases is still in its infancy. Nanotechnology has the potential to play a critical role in global food production, food security, and food safety. The applications of nanotechnology in agriculture include fertilizers to increase plant growth and yield, pesticides for pest and disease management, and sensors for monitoring soil quality and plant health. Over the past decade, a number of patents and products incorporating nanomaterials into agricultural practices (e.g., nanopesticides, nanofertilizers, and nanosensors) have been developed. the use of nanoscale nutrients (metals, metal oxides, carbon) to suppress crop disease and subsequently enhance growth and yield. Notably, this enhanced yield may not only be directly linked to the reduced presence of pathogenic organisms, but also to the potential nutritional value of the nanoparticles themselves, especially for the essential micronutrients necessary for host defense. but high toxicity of nanoparticles inadvertently released in the environment may pose greater threat to man and other organisms. Therefore, nanotechnological progress is to be viewed with caution and dealt accordingly. The collective goal of all of these approaches is to enhance the efficiency and sustainability of agricultural practices by requiring less input and generating less waste than conventional products and approaches.

Keywords: plant diseases, nanotechnology, crops

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Preparation of Novel Green Nano Catalyst and Survey Its Properties

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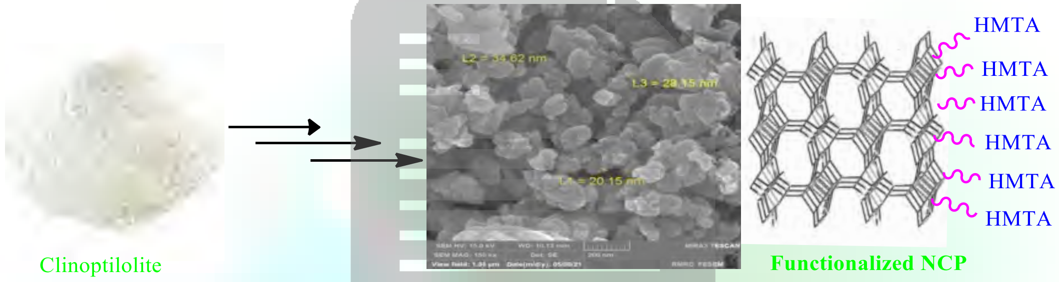
Graphical Abstract



Abstract: Recently, the development of environmentally benign and clean synthetic procedures has become the goal oforganic synthesis. Green chemistry is a rapidly developing new field that provides us with a proactive avenue for the sustainable development of future science and technologies. Green chemistry uses highly efficient and environmentally benign synthetic protocols to deliver lifesaving medicines, accelerating lead optimization processes in drug discovery, with reduced unnecessary environmental impact. Catalytic approaches might be considered as green since specific chemical transformation could be achieved within very short time with the addition of very little catalysts, significantly reducing production cost aswell as health and environmental risks [1-3]. Due to the importance development of green chemistry, in this research we wish to report green synthesis of novel, efficient, low cost, environmentall friendly with high reusability catalyst using clinoptilolite, and its catalytic application for green synthesis of Mannich bases on the base of coumarin in addition of other applications of this product in green industrial. The structure of novel nano synthetic catalyst confirmed by variouse techniques such as XRD, FE-SEM, EDS and FT-IR.

Keywords: Green, Nano Technology, Synthesis, Novel, Coumarin.

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Extraction of Thymoquinone from Blackseed with Electrospun Nanofibers as A New Method and Detection of It with Electrochemical Biosensor

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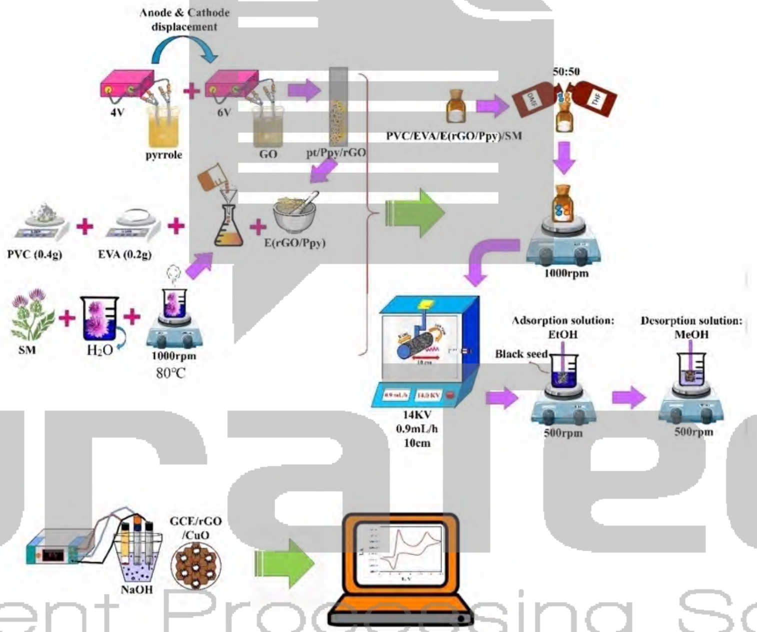
Graphical Abstract



Abstract: Thymoquinone is the main constituent of blackseed and it has effects on the treatment of many illnesses such as kidney diseases **[1]**. Because of thymoquinone advantages, First, new electrospunnanofibers with polyvinyl chloride/ethylene vinyl acetate Latex /Electrochemically (reduced graphene oxide/polypyrrole)/Silybum marianum inflorescence extract (PVC/EVA/(rGO/Ppy)/SM) was prepared, and then thymoquinone was extracted from Nigella

Sativa with these nanofibers. Finally, detection of Thymoquinone was done with the construction of a simple nonenzymatic electrochemical biosensor with using the Copper (II) oxide nanoparticles/reduced graphene oxide/glassy carbon electrode (CuO/rGO/GCE). The otrGO has large surface area **[2]** and strong mechanical properties. Other electrochemical methods for studing of the TQ need to more time [3]. The effective conditions on TQ adsorption and desorption were optimized by Design-Expert 12.0 software and one at time method, respectively. Also, time and potential values that were effect on constructed biosensor were optimized by both Design-Expert 12.0 and one at time methods and the comparison between two methods was done. So the optimized factors are: time of reduction of GO to rGO = 120 s, Cu deposition potential and time = -0.25 V and 250 s, respectively. The morphology of PVC/EVA/(rGO/Ppy)/SM nanofibers and nanocomposites that was used for electrode modification were characterized by field emission scanning electron microscopy and EDAX-elemental mapping analysis. The structure characterization of electrospun nanofibers was done by Fourier transforms - infrared (FT-IR) Spectrometer, X-ray diffraction (XRD), and thermogravimetry analysis (TGA). Also, the nanocomposite structure was investigated by Raman spectroscopy, XRD, ultraviolet-visible (UV-vis) spectroscopy, and FTIR. The conductivity of GCE and GCE/rGO/CuO electrode surfaces was compared with electrochemical impedance spectroscopy (EIS). Finally, the electrochemical biosensor was put into human blood serum samples and the standard addition method was done with the addition of TQ standard solution to them. The linear range and detection limit was reached 50-1000 µM and 4.85 µM, respectively (S/N=3).

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The Aggregation Behavior of Ion-Pairs in $[MIM^+]_2[C(CN)_3^-]_2$ Ionic Liquid: A Theoretical Study

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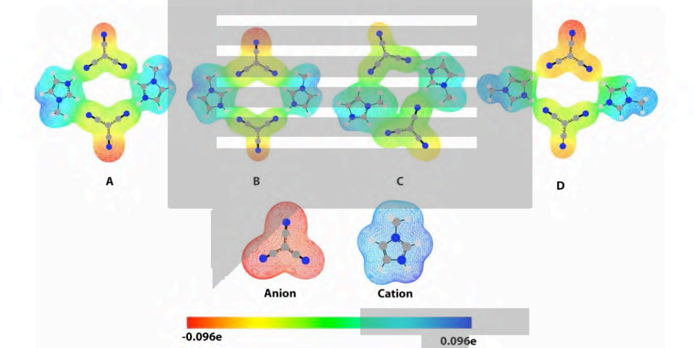
Graphical Abstract



Abstract: The use of toxic and hazardous organic solvents is oneof the most important problems in the chemical industry.Therefore, there is a fundamental need to find out areplacement for the toxic solvents used in the chemicalprocesses [1-3].The most important alternatives to toxic solventsare ionic liquids. Ionic liquids (ILs) are salts with meltingpoints below 100 ºC, which can replace toxic organicsolvents in a range of well-known processes [4]. Theexistence of microstructures or clusters in ILs is animportant characteristic of many ILs and provides importantinformation to better understand IL applications in various fields [5]. In the present work, the aggregation behavior of ion-pairs in $[MIM^+]_2[C(CN)^-_3]_2$ ionic liquid was investigated. The quantum chemicalcalculations were carried out to determine the structural parameters, interaction energies, hydrogen bonding, physical and topologicalproperties of the clusters formed in the ionic liquid of $[MIM^+]_2[C(CN)^-_3]_2$. The solvent effect on the stability of clusters was examined.

TheGibbs free energy of solvation and the Gibbs free binding energy of clusters in various solvents were calculated. The results show that withdecreasing the polarity of the solvent, the tendency to the formation of aggregate increases. Also, the solvation energies of the clustersincrease with decreasing the solvent's dielectric constant. The NBO analysis was performed to evaluate the charge transfer in complexes.

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An Electrochemical Platform Based on CuO/N-rGO Nanocomposite and IL for The Determination of 2-Aminophenol

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Abstract: In last decade, the protection of environment from the pollution is global concern. [1]. 2-amino phenols are aromatic compounds contains amino and hydroxyl group adjacent to each other on benzene ring, they are good reducing agents, chemically reactive and amphoteric in nature. 2-amino phenols are possessing toxic effects because of its easy penetrating property into the skin, membranes of plants and animals causes genotoxic, mutagenic and hepatotoxic effects. In the recent years, nanomaterials based electrochemical sensors have found a lot of utilizations due to their unique properties. The unit features such as larger ratio of the surface to volume involve in higher sensitivity and new sensing features of nanomaterials. Furtheremore, ionic liquids (ILs) are widely employed in electroanalysis, particularly for designing sensors based on the electrode modifications due to their unique features, including lower volatility and higher ionic conductivity [2]. In this work, we reported the electrochemical sensing of 2-aminophenol by using a carbon paste electrode (CPE) modified with CuO/N-doped reduced graphene oxide (CuO/N-rGO) nano-composite and IL. The prepared sensor has outstanding performance in the determination of 2-aminophenol with higher sensitivity, wider linear ranges, and a lower limit (0.03 µM) of detection.

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A Review of NiSe-Based Electrocatalysts as Highly Efficient Electrocatalysts for Water Splitting

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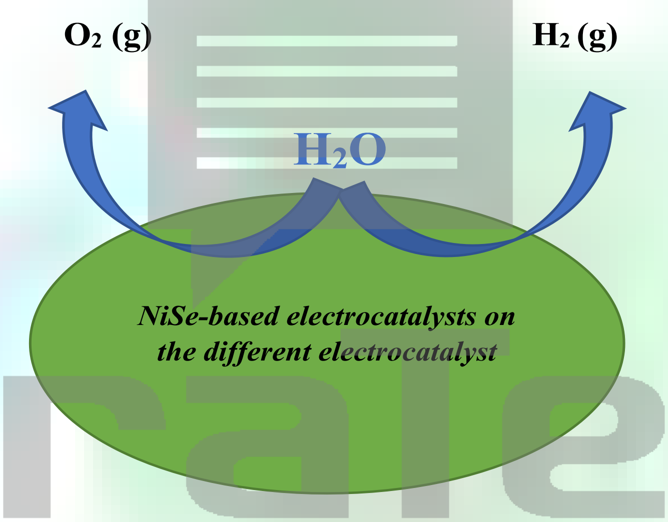
Graphical Abstract



Abstract: Water splitting, as an advanced energy conversion technology, consists of two half-reactions, including oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). However, the ideal electrocatalysts are noble metal-based catalysts. Their high cost and scarcity on earth seriously restrict the large deployments. NiSe-based materials have attracted significant attention due to their excellent catalytic properties for OER and HER. Nevertheless, their conductivity and electrochemical stability at high current density are unsatisfactory, resulting in ineffective water splitting due to high impedance and low stability. Recently, a series of catalysts coating NiSe-based materials on the different substrates such as 3D nickel foam and carbon cloth and other substrates were extremely stable under the circumstance of high current density.

There are several meaningful reviews about the NiSe-based electrocatalysts and the electrocatalysts on 3D nickel foam, carbon cloth, and other substrates. However, no systematic

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review about the combination of them for OER and HER has been reported yet. Therefore, in this review, we summarize the reports of NiFe-based catalysts on nickel foam in OER and HER, respectively. This review will provide a more comprehensive understanding of NiFe-based electrocatalysts on 3D nickel foam, carbon cloth, and other substrates and give some references for the design of such electrocatalysts in the future.

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Application of BC_2N Nanotubes as A Sensor in The Adsorption of CN Radicals

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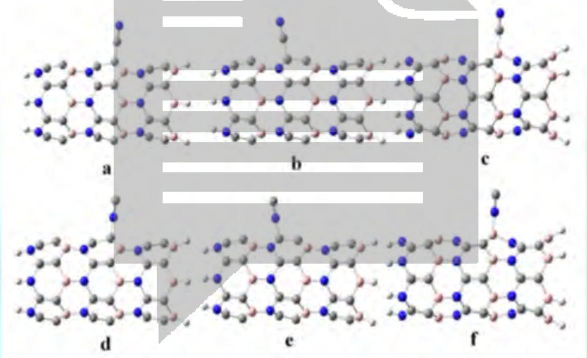
Graphical Abstract



Abstract: Air pollution by gas molecules threatens the life and health of the human beings on the planet in many ways [1]. Carbon nanotubes are porous materials with a high reactivity exterior surface, which makes them sensitive to molecular adsorption [2,3]. The electronic structures and transport properties of CNTs can be modified by mechanical deformations; doping or topological defects. Substituting CNTs with other elements like B and N can tune their electronic properties efficiently and lead to novel applications. Among various $B_xC_yN_z$ systems, the BC_2N is believed to be one of the most stable stoichiometries [4]. The CN radical is an important molecule due to its role in combustion chemistry and atmospheric chemistry. The chemistry of cyanide is also important to understand the surface chemistry of C- and N-containing systems. this work, we have investigated the adsorption behavior of the CN radicals on electronic properties of BC_2N nanotube (BC_2NNT) by B3LYP/6-31G(d) method. The results show that CN radicals can be chemically adsorbed on the nanotube. Based on the energy analysis, the most stable position of CN radical on the nanotube is C1 site. Also, the C-side complexes are more stable than the N-side complexes.

We investigated the effects of CN radicals adsorption on the electronic properties of the BC_2N nanotube. According to our calculations, band gap energy of the BC_2NNT decreases with increasing the number of CN radicals. It is predicted that the conductivity and reactivity of nanotube increase by increasing the number of CN radicals. Based on the NBO analysis, in all complexes charge transfer occurs from nanotube to CN radical. The AIM results show that, the $X_{tube}\ldots Y_{CN}$ interaction has covalent nature. Generally, The BC_2N nanotube can be used to as sensor for nanodevice applications.

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Application of Prepared Nickel Oxide Nanoparticles in Treatment of Contaminated Water

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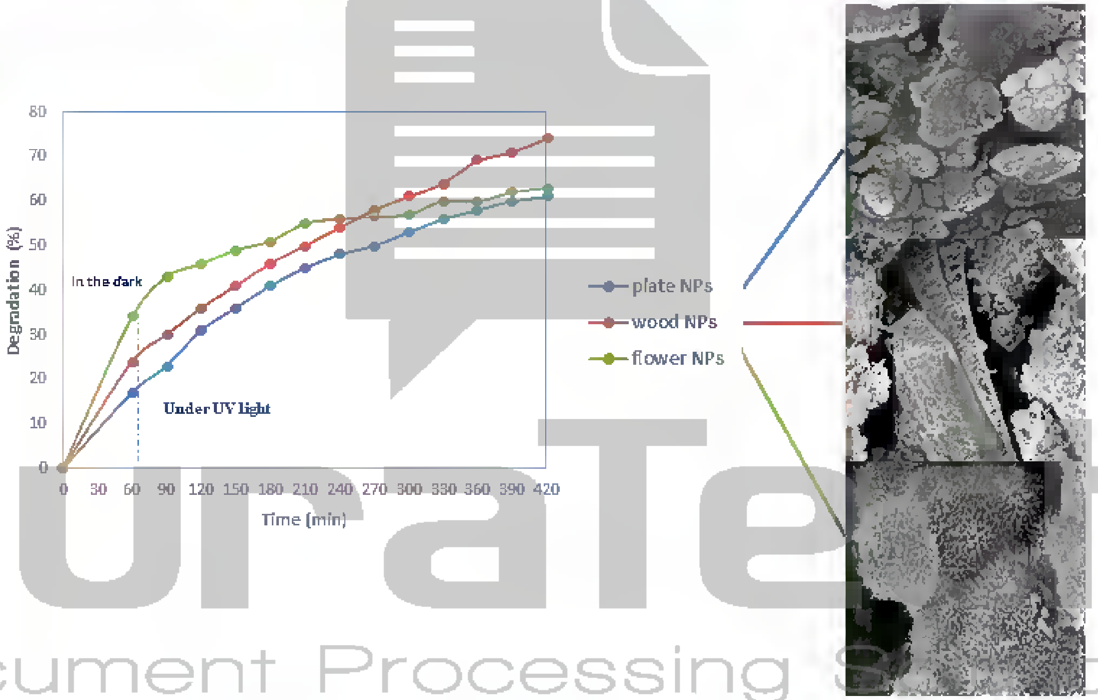
Graphical Abstract



Abstract: In the present study, NiO nanoparticles (NPs) were synthesized with nano-plate and nano-flower morphologies by hydrothermal method and nano-wood morphology by sol-gel method[1,2]. The crystal structure, morphology, and particle size of the synthesized samples were examined using X-ray diffraction (XRD) and scanning electron microscopy (SEM) techniques. The photocatalytic properties of synthesized nanoparticles in the removal of Direct Red 23 (DR-23), as a sample of dye contaminants, were investigated using UV-Vis spectroscopy technique. Removal of DR-23 from aqueous solution was investigated using adsorption and photocatalytic activity of NiO NPs in the form of plate, flower, and wood morphologies. The results showed that the dye removal percentage(R) in the presence of plate and wood NiO NPs (initial

dye concentraion= 50 ppm, catalyst dose= 300 ppm) were 17% and 24% in 60 minutes of darkness, and after 6 hours radiation of ultraviolet (UV) light reached to 61% and 74%, respectively. Also, the performance of flower morphology of NiO was investigated with two doses of 300 and 100 ppm. The removal percentages were obtained 100% and 34% in the darkness, respectively. Also, when 100 ppm nano-flower NiO was irradiated under UV light the removal percentage increased to 63%. Therefore, NiO NPs with flower morphology have the best efficiency in degradation of DR-23 dye at pH = 5.5 under UV light (R=63%, catalyst dose= 100 ppm, dye concentration= 50 ppm).

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Equilibrium, Kinetics and Thermodynamic of Methyl Orange Adsorption ontoThe Chitosan/Montmorillonite Nanocomposite

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Abstract: Chitosan-montmorillonite (CTS–MMT) was used as an effective adsorbent for the adsorption of anions. In this research, the adsorption of methyl orange dye as an anionic sulphonated azo dye, from aqueous solution by CTS–MMT nanocomposite was investigated. The synthesized nanocomposite was characterized by FTIR (Fourier transform infrared), XRD (X-Ray diffraction) and SEM (Scanning Electron Microscopy) to evaluate the morphology. Adsorption experiments were performed at room temperature in batch system. The effects of pH, initial concentration of dye, contact time and adsorbent dose were studied. Kinetic and equilibrium sorption parameters were evaluated pseudo-first and pseudo-second rate models and Langmuir and Freunlich equations. The results indicated that the adsorption of methyl orange dye onto CTS-MMT can be best described by pseudo second-order model. Also, the adsorption data well fitted to Langmuir and Freundlich isotherms.

Keywords: Adsorption kinetics, Isotherms model, Chitosan–montmorillonite nanocomposite, methyl orange, Thermodynamic parameter

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Application of A Synthetic Ligand in Rapidly Synergistic Cloud Point Method for Separation and Preconcentration Trace Amounts of Copper of Water Samples

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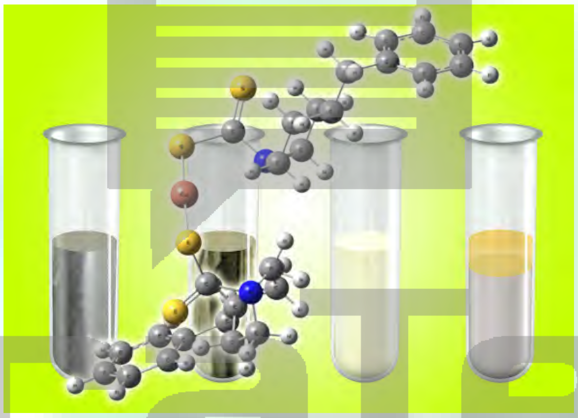
Graphical Abstract



Abstract: In recent years, the presence of heavy metals in wastewater has been a major environmental problem due to its properties such as solubility, reduction-oxidation, complex formation, accumulation, non-degradability, and stability [1–3]. Copper is used in industry and agriculture and its presence is essential for plant and human health, but excessive consumption can also be harmful to health. The amount of copper in water depends on pH, the concentration of carbonate, and other water-soluble anion. Several methods including atomic absorption spectrophotometry [4, 5], differential pulse anodic stripping voltammetry [6], luminescent [7], inductively coupled plasma [8] and Ultraviolet-visible spectrophotometry have been applied for the determination of copper. Uv-vis spectrophotometry can be used due to ease of operation, inexpensive materials, and easy access. For measuring copper at very low concentrations in complex matrices were used pre-concentration techniques such as liquid-to-liquid extraction [9], membrane extraction [10], solid phase extraction [11], solid phase microextraction [12], liquid-phase micro-extraction [13], and cloud point extraction [14]. The rapidly synergistic cloud point extraction (RS-CPE) technique was first proposed in 2011 by Wen et al [15, 16]. In this study, a

rapidly synergistic cloud point extraction method was used to separate and pre-concentrate small amounts of copper ions. Synthetic ligand 4-benzylpyridine dithiocarbamate as a complexing agent, non-ionic surfactant (Triton X-100) as an extractant, and octanol as a synergic reagent were used. Parameters affecting copper ion extraction such as pH, ligand concentration, octanol volume, type of diluent solvent, stirring speed and time, surfactant concentration, and the effect of ionic strength were investigated. Ultra violet visible spectrophotometry was used to measure the absorption of copper complex. Under optimal conditions, limit of detection, preconcentration factor, and relative standard deviation for copper were 1.4×10^{-3} µg /mL, 10 and 2.1, respectively. Also, the relative extraction efficiency of copper extraction in real samples was greater than 97%.

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Determination of Polycyclic Aromatic Hydrocarbon (PAHs) in Soil and Plant Samples

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Abstract: Environment pollution to dangerous and poisonous chemical substances is one of the major problems which industrialized world counters with. Among pollutants exists in environment, persistent organic pollutants (POP), polycyclic aromatic hydrocarbon (PAHs) In case of existence in food chain, polycyclic aromatic hydrocarbons are one of the most worrying indices and threats for living things. Vegetables are one of the most important food resources and provide main part of energy, cellulosic substances, and vitamins which are necessary for people. Therefore, planting and developing them is really important. Moreover, such products must be provided carefully according to their importance and usage.

Kerosene usage in some farms in Khuzestan Province such as Dezful, Safi Abad as herbicide leads to soil and vegetables pollution specially carrot in these farms. Kerosene density increase leads to polycyclic aromatic hydrocarbons in soil and plants. It also increases the density of zinc, copper, lead and cadmium significantly in roots and other parts of vegetables. The current research aims to measure petroleum pollutant and also heavy metals in soil and plants sample. in order to extract the polycyclic aromatic hydrocarbons and Aliphatic hydrocarbons in plants and soil samples, Soxhlet extractor and coupledQuEChERS with ultrasonic were used. And in order to measure the PAHs amount, Gas chromatography- Mass Spectroscopy (GC-MS) were used. All the elements exist in soil sample were set by dissolution method with Hydrofluoric acid and Perchloric acid according to ISIRI 11115_1 1st. edition standard and Mass Spectroscopy machine- inductively coupled plasma. Lead, cadmium, copper, zinc, and ferrum amount in plant samples were measured by graphite furnace atomic absorption spectroscopy after microwave digestion. Due to volatility of petroleum compounds such as aromatics, dry freeze method was used to dry samples instead of dry oven method.

Findings reveal that suggested coupled QuEChERS method with ultrasonic followed by DLLME purification and GC-MS analysis is perfectly able to set very little amount of PAHs in plants and soil samples. According to qualified numbers comparable to other methods, we can point to its good function. The relative standard variation based on six times measuring for 16 PAH is between 3.8-3.10% and for TPH is between 97.8-30.10%, the recognition limit of 0.01 – 0.16 ng/g for PAH and 8.97-10.30 for TPH and set limit amount 0.97-6.34 for PAH and 0.13-0.98 ng/g for TPH.

Keywords: polycyclic aromatic hydrocarbons (PAH), GC-MS, QuEChERS. Soil, Plant. HPLC, Kerosene. Heavy Metal

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Nazar Abad industrial Park Wastewater Treatment Using Plasma/Fenton process

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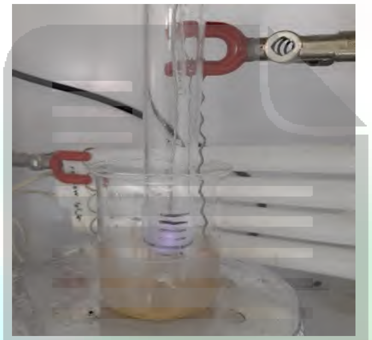
Graphical Abstract



Abstract: There are various methods for water and wastewater treatment; however, each one has its own advantages and disadvantages. In recent years, plasma technology as one of the advance oxidation processes (AOPs) has received a lot of attention for industrial wastewater treatment due to high efficiency, no secondary pollution, eco-friendly and low cost. Furthermore, Fenton process as another AOPs has been widely used in industrial wastewater treatment. In this project, the performance of the combined plasma-heterogeneous Fenton (Plasma/Fenton) process in treatment of wastewater treatment was investigated. Magnetite was synthesized as the heterogeneous catalyst of Fenton. Chemical oxygen demand (COD) was used to measure the concentration of pollutant in the wastewater and the amount of its removal efficiency. According to the obtained result, the efficiency of plasma/Fenton process was enhanced by magnetite dosage up to 0.2 g, plasma power up to 35 kW and oxygen flow rate up to 0.5 L/min. The plasma/Fenton had ability to reduce the effluent of the industrial town more than 90%. Furthermore, the performance of the plasma/Fenton was higher than individual plasma and Fenton processes.

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Electrochemical Carwash Wastewater Treatment by A New Flow Cell System

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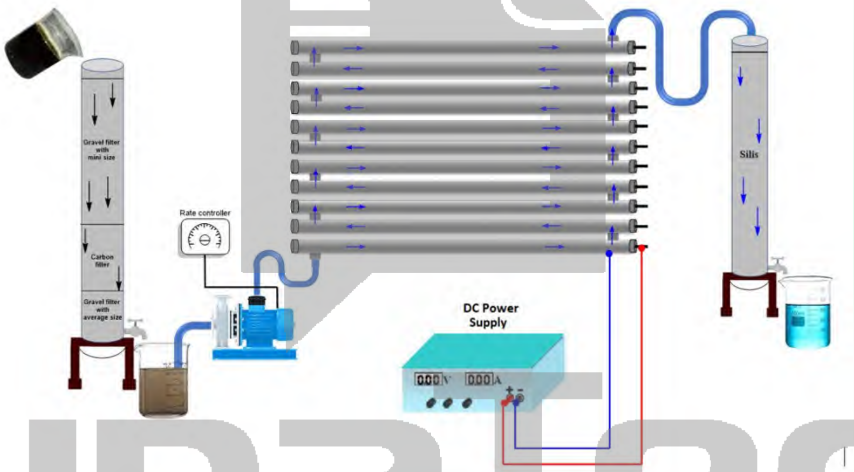
Graphical Abstract



Abstract: Nowadays water is an important issue and water scarcity is one of the main problems around the world. One of the main ways to solve the problem is wastewater treatment. Water treatment has different methods, such as chemical processes, advanced oxidation, biological and enzymatic treatment [1]. One of the most important methods of water treatment is electrocoagulation process. It is an electrochemical method for the production of coagulants and removing colloidal material, metals, suspended solids, pesticides and also harmful microorganisms from water and wastewaters. In this method, a direct current is applied to a sacrificial anode (mostly Fe or Al).This process (electrodissolution) increases the concentration of the metal iones (Al^{3+}or Fe^{3}) in solution, and these ions are eventually converted to oxides and hydroxides[2-4]. This method has been used by many scientists in recent years due to its many advantages such as cheapness, availability and being safe for environment. In this research, wastewater treatment has been performed by designing a new flow system for carwash wastewater treatment. It consists of: (I) a column filled with activated carbon and sand in order to filtration of large and suspended particles of

wastewater, (II) an tunable pump, (III)a tubular flow electrochemical rector consisting of iron cathode and aluminum anode which are connected to a DC power supply. This reactor is the main part of the package. (IV) a column after reactorfilled withsandin order to remove of generated flocks. In this research, the effective factors such as current density, flow rate, electrolysis time and electrodes material, have been optimized. The 88% reduction of COD obtained with this package during a single pass through the system. The treated wastewateris odorless, colorless and clear and can be used in agricultures and industries.

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Activated Carbon Decorated with Grape Stalks Powder for Methylene Blue Adsorption from Aqueous Solutions

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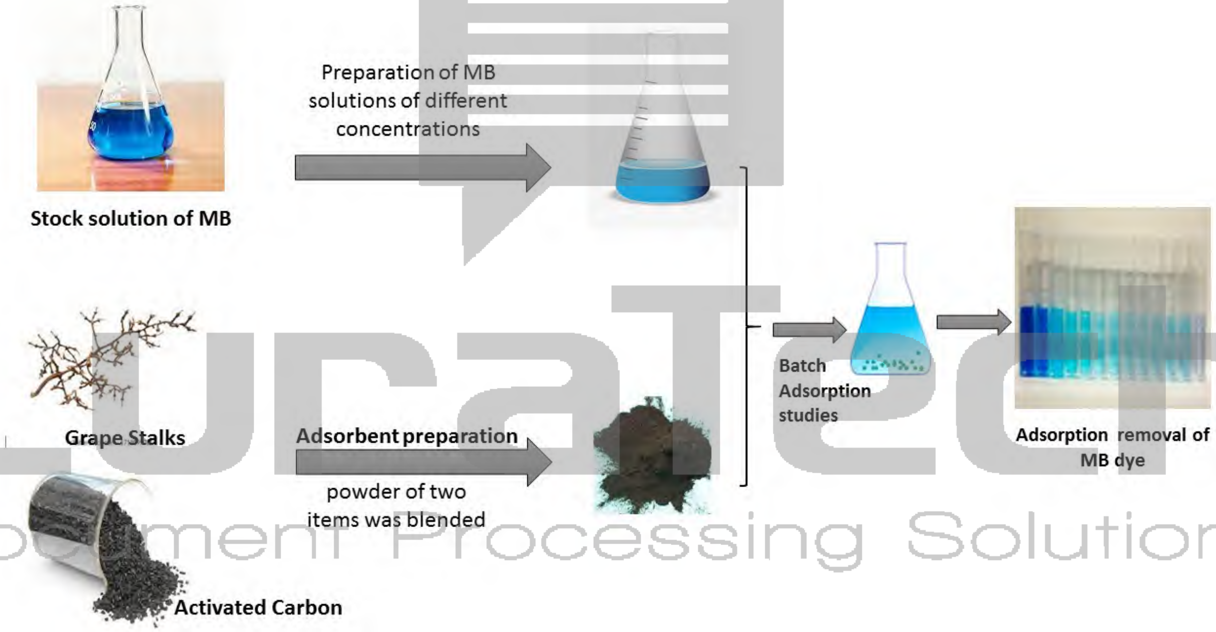
Graphical Abstract



Abstract: In this study, activated carbon was combined with grape stalks powder to adsorb methylene blue (MB) dye with various concentrations from a wastewater. Five independent items including pH (2–13), contact time (5–270 min), grape stalks powder dosage (0.1–10 g/ l), methylene blue initial concentration (20–300 mg/l), and activated carbon dosage (0.1–10 g/l) in methylene blue adsorption process were investigated. The Central Composite Design (CCD) under Response Surface Methodology (RSM) was applied to assess the independent variables effects on the methylene blue adsorption. The pseudo-first order, pseudo-second order, Elovich and intraparticle diffusion models were employed to study the adsorption process kinetics. The Langmuir, Freundlich, Temkin and Dubinin-Radushkevich isotherm models were applied to consider the adsorption isotherm. It was concluded that the intraparticle diffusion isotherm and pseudo-second order kinetic models could show the best results in this research and The Langmuir isotherm modelcould validate the adsorption process isothermal behavior which was monolayer and homogeneous.Pursuant to the Freundlich model data, grape stalks powder blended withactivated carbon was an great adsorbent for the MB adsorption because 1/n was equal to0.1672 ($0 < 1/n < 1$ for an excellent adsorbent).The data analysis indicate that the adsorbent capacity was dramatically increased for the activated carbon (as base adsorbent) blended with grape stalks powder. In addition, some data such as physical adsorption (by analyzing FTIR and applying some standard equations) and mean free energy (E=0.572) were discovered, as well. Finally, activated carbon decorated with grape stalks powder was found as an eco-friend adsorbent for the methylene blue (and the other cationic dyes) reduction from aqueous wastewaters.

Keywords: Adsorption, Biomass, Methylene blue, Wastewater.

A heterogeneous Catalyst for Synthesis of Arylbenzothiazoles from Aldehydes

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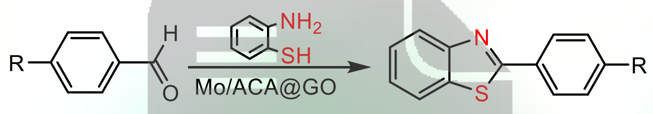
Graphical Abstract



Abstract: Benzannulated heterocycles such as benzothiazoles are very important intermediates in organic reactions [1]. Several methods have been developed for the preparation of these heterocycles including the condensation of aldehydes [2], amides [3], or carboxylic acid derivatives [4] with o-amino thiophenols. The development of efficient and environmentally benign chemical processes or methodologies for widely used heterogeneous recyclable catalyst under solvent-free conditions are one of the major challenges for chemists in organic synthesis. Herein, we wish to report a polyoxometalate- modified graphene oxide hybrid heterogeneous catalysts were synthesized by the reaction of $MoO_2(acac)_2$ with graphene oxide functionalized by grafting procedures of (3-chloropropyl) trimethoxysilane and aminopolycarboxylic acid, respectively. The as-synthesized catalysts were effective in the catalytic in the preparation arylbenzothiazoles. Moreover, the reusability of the catalyst was excellent and the leaching of heterogeneous catalyst was dramatically suppressed. High yields, short reaction times, eco-friendly conditions, simplicity of the procedure, reusability of the catalyst and broad substrate scope are the merits of this protocol.

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A Green Approach for The Electrochemical Dimerization of Edaravone

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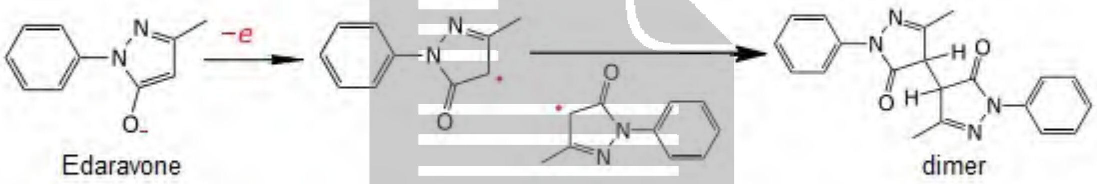
Graphical Abstract



Abstract: Edaravone is a free radical scavenger and neuroprotective agent used for the treatment of acute ischemic stroke and Amyotrophic Lateral Sclerosis (ALS) [1]. Edaravone and its derivatives are also renowned for their antitumor and hypoglycemic activities. Edaravone has attracted the attention of many chemists due to its antioxidant property and free radical scavenging activity [2]. In this work, a green electrochemical method for the synthesis of new dimer of edaravone is described. The electrochemical behavior of edaravone has been investigated in detailed at different pHs regions by cyclic voltammetry and coulometry. Cyclic voltammograms of a edaravone shows an anodic peak, which correspond to the transformation of edaravone to corresponding radical, through an irreversible one electron process. This could be considered as a criterion for the instability and reactivity of radical that is produced at the surface of electrode [3]. The electrochemical synthesis has been successfully performed in an undivided cell using graphite electrode without toxic reagents and solvents using an environmentally friendly method.

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Standardization of Dispersive Liquid-Liquid Microextraction for Determination of 16 Polycyclic Aromatic Hydrocarbons in Water Samples

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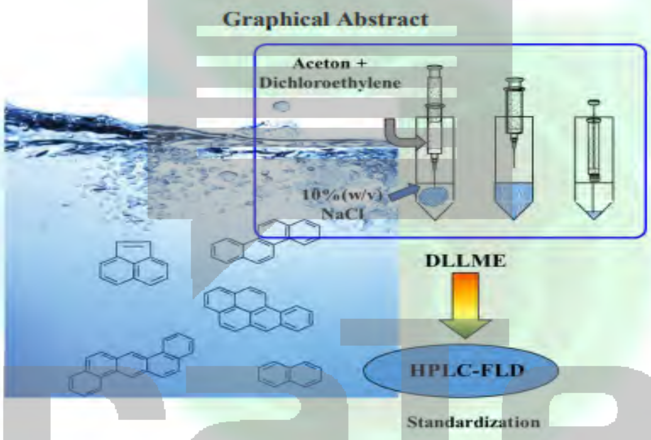

Abstract: In this study, Dispersive liquid-liquid microextraction (DLLME) combined with high performance liquid chromatography-Multichannel Fluorescence detector (HPLC-FLD) as a simple, fast and inexpensive method have been optimized in order to develop a standard method for determination of polycyclic aromatic hydrocarbons (PAHs) in water samples. In the optimum condition, 6mL of extraction mixture contains aceton (disperser solvet) and dichloroethylene (extractor solvent) (50:1) are rapidly injected into the sample (30.00 mL) containing 1 mL of NaCl solution (10 w/v%). Therefore, a cloudy solution is formed. After centrifuging, the sedimented phase were transferred into a vial and evaporated at 35°C under nitrogen atmosphere. Thereafter, 200 µL acetonitrile is added to the vial, the obtained solution evaluated using HPLC-FLD. Under the optimum condition, it was possible to measure 14 PAHs compounds. The linear ranges for most compounds are in the range 0.5-0.5 µgL-1. The recovery rate is between 65% -94% and the quantitative detection limit (LOQ) is in the range of 0.003-0.12 µgL-1. The relative standard deviation (RSD%) in the concentration of 0.7 µgL-1 of PAHs were 4.5-7.7% (n=3). The method was validated by simultaneous testing of a spiked sample with the standard method (ISIRI 9387-2) and the mean results were compared using t-test. The extraction method was also coupled with

gas chromatography-Mass spectrometer (GC-MS) to evaluate its performance and robustness. Finally, the optimized method was used to measure the concentration levels of PAHs in 40 water samples. The proposed procedure is can be developed to determine PAHs in other matrices. In order to standardization the method, its precision including repeatability and reproducibility, accuracy and robustness were tested.

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Use of TiO_2 Nanoparticles as Air Cathode Modifier in Rechargeable Lithium-Air Batteries to Improvement of Performance

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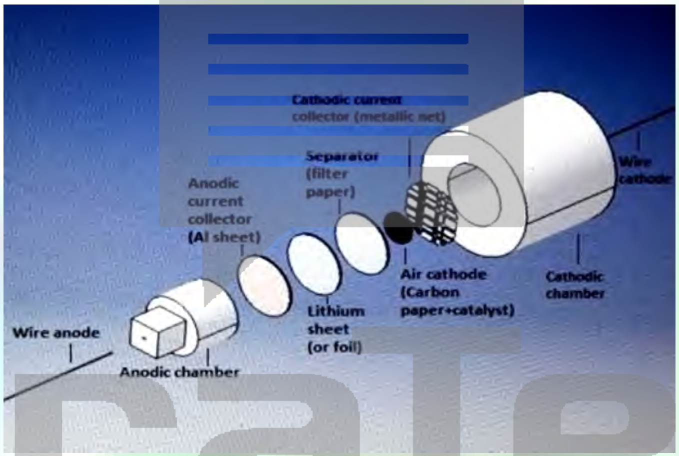
Graphical Abstract



Abstract: Today, Li-O_2 rechargeable batteries are the most attractive energy storage devices used for electric vehicles because to their high energy density. A Li-O_2 battery is composed of an air cathode, electrolyte containing Li, and Li metal as an anode. However, there are many limitations for this batteries, such as short cycling life, capacity and lifetime more due to the deposition of the insulated Li_2O_2 (as discharge product) on the cathode pore leads to fading capacity and a high overpotential. It is found that the developing catalyst such as transition metals, transition metals oxide and noble metals in these batteries cathode for O_2 electro-reduction process is the one effective key to improving battery performance and to overcome many cathode limitations. For this reason, TiO_2 is an attractive electrocatalyst with excellent electrochemical activities due to its high stability, unique physicochemical properties. This work aims to observe the electrochemical performance of TiO_2 as an air cathode modifier. However, TiO_2 nanoparticles were synthesized via the facile sol-gel method and investigated as air cathode modifier in lithium-air batteries. The

phase structure, surface morphology, and elemental composition of the synthesized TiO2 nanoparticles were characterized as well. Additionally, the TiO2 as nanocatalyst was deposited on the cathode carbon sheets, and their electrochemical performances of lithium-oxygen were evaluated via an ECC-Air test cell using cyclic voltammetry, electrochemical impedance measurements, and galvanostatic charge-discharge tests. Consequently, the air cathode containing TiO2 showed a full discharge capacity of 2000 mAh/g and a specific capacity of 500 mAh/g for 120 stable cycles. Interestingly, the discharge potential increases from 2.35 V to 2.90 V and so the overpotential amount of the battery was decreased.

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Facile Extraction of Coomassie Brilliant Blue G into Nanovesicles of Octanoic acid as a Fantastic Green Supra Molecular Solvent Phase

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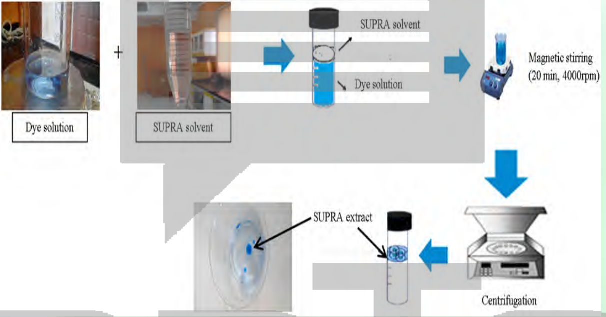
Graphical Abstract



Abstract: The separation of polluting dyes from economical and industrial wastewaters is so important. Liquid-liquid mico-extraction is a kind of separation methods for pollutant removal from aqueous samples. Since organic solvents are toxic and flammable, nowadays, the substituting of green solvents is one of interest. So, supramolecular solvents (SUPRAs) can be a good candidate in liquid-liquid micro-extraction methods. SUPRAs have some advantages in comparison with other organic solvents, such as: friendly environment, not flammability, and high extraction efficiency in low volumes.

In this research, supramolecular solvent containing nanovesicles of octanoic acid (SUPRA) was synthesized and tetrabutyl ammonium hydroxide was used as coacervating agent. The characterization of nanovesicle aggregates in SUPRA phase was proved by dynamic light scatterig spectroscopy (DLS). Then, produced SUPRA was used as green separating liquid phase to extract Coomassie Brilliant Blue G (CBBG) from aqueous samples. Also, the effective parameters on dye extraction, such as: the concentration, volume, temperature, and pH of dye solution, separation time, types of aggregates in SUPRA phase and volume of liquid SUPRA phase, were investigated. Under optimal conditions: 50 ml of 2 ppm (CBBG) at pH=5.4 in ambient temperature (25°C), about 93%±0.063 (n=10) of dye was extracted into 355µl of SUPRA in 20 min of extraction time. Pre-concentration factor was obtained about 140.84. Also the effects of matrices were investigated and the results showed that, under optimal conditions, quantitative amount of dye could extract into 355 µl of SUPRA phase after 20 min from Korouz company wastewater, Karaj river water, and Shahr-e-Qods drinking water. Therefore, there was no significant interfering effect on dye removal and also dye could be separated easily and in a short time (20 min) into low volume of environmentally friendly SUPRA phase (0.355 ml).

Keywords: Green supramolecular solvent, Coomassie Brilliant Blue G, Liquid-liquid microextraction, Nanovesicles, Octanoic acid.

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Safe and Environmentally Synthesis of a Co (II) Nano Coordination Polymer

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Abstract: In the last two decades, immense attention has been paid to the reactivity of nano coordination polymer for the sake of environmental reasons and its abundant, safe, inexpensive, and nonflammable features as a C building block for organic chemistry. Heterocycles are one of the most privileged families of organic compounds that constitute an extensive number of natural products and display a broad range of pharmaceutical and biological activities. Therefore, synthetic chemists continue to be interested in the preparation of these compounds. Despite wide importance of heterocyclic in pharmaceutical and biotechnology industries, safe, non-toxic, and highly efficient synthesis of these compounds still remains to be a difficult problem. In this study, we have highlighted the advances in this chemistry which will be helpful in the development of improved methods for the convenient and green synthetic pathways for the construction of bithiazole nano coordination polymers. This new page of bithiazole nano coordination polymers synthesis plays an important role in green and sustainable chemistry. In our work, nanostructures were synthesized by the one pot microwave process via solid state reaction at low temperature as a way for green chemistry method. This method of preparation may have some advantages such as: it takes place with shorter reaction times, produces better yields and it also is likely to produce nano-sized particles of the coordination compounds. The nanostructures were characterized by scanning electron microscopy (SEM), X-ray powder diffraction (XRD), Infrared spectroscopy (IR), ^{1}H, ^{13}C -NMR spectroscopy and elemental analyses. The new bithiazole was further characterized by UV-visible spectrophotometric measurements. The thermal stability of compound both its bulk and nano-size has been studied by thermal gravimetric (TG) and differential thermal (DTA) analyses. Synthesis of bithiazole nano coordination polymer, making use of this method, is a novel approach in the literature.

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Determination of Lead with rGO/MoS_2 Nanocomposite-Based Electrochemical Sensor

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Abstract: In this work, rGO/MoS_2 were fabricated on screen-printed electrode (SPE) substrates by developing a simple electrochemical deposition and annealing method. The as-prepared rGO/MoS_2 nanocomposite were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), and infrared spectroscopy (IR). Heavy metals require careful monitoring due to their toxicity, and current methods are too complex or bulky for point-of-care use[1]. Electrochemistry offers a convenient alternative for metal determination. The differential pulse voltammetry (DPV) method was performed to determine target metal ion. The effects of different experimental variables such as supporting electrolyte type and pH were investigated and optimized. At optimal electrochemical conditions, the developed electrode exhibited linear voltammetric responses in the ranges of 0.2–5.4 µM with the detection limits of 0.12 µM. In addition, the effects of common cation and anion interferences commonly found in environmental water were studied, and the satisfied results were obtained. Furthermore, the method was successfully applied to the determination of target analytes in lake water samples and satisfactory recoveries were observed from different spiked values.

Keywords: Metal monitoring, Electrochemical sensor, Reduced graphene oxide, Molybdenum disulfide

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The Investigation of Modification Methods, Kinetic and Ammonia Adsorption by Iranian Clinoptilolite Zeolite

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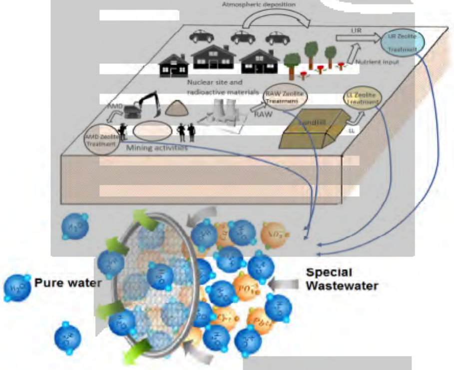
Graphical Abstract



Abstract: In this study, Iranian clinoptilolite zeolite was investigated for removal of ammonium. Here efficacy of both zeolite and modified zeolite by chemical methods were investigated. The zeolite was modified using $FeCl_3.6H_2O$ 0.2 M, sodium hydroxide 4M for 72 h and HCl 0.5 M. Characterization of the prepared adsorbent was carried out using various techniques such as XRD, FESEM, EDS and BET analyses. Experiments with aqueous solutions containing concentrations of ammonium ion (2000 mg/ L) by contacting certain amounts of natural clinoptilolite (0.001-0.1) gr, for (5- 240) min and in different pH (2- 10.5) were investigated.The maximum amount of ammonium uptake for natural zeolite at a concentration of 2000 mg/L was obtained at pH = 8.5 with 0.1 g of natural zeolite for 1 hour. The results show that the highest amount of ammonium uptake by the HCl-modified zeolite was about 1999 mg/L. Also, the results indicate that the HCl-

modified of Clinoptilolite could provide strong basic sites and mesopore structure (average pore diameter of 5.8803 nm) with high surface area (40 m^2 g^{-1}) for removal of ammonium up to 99%.

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Determination of Polycyclic Aromatic Hydrocarbons in Soil, Tree Leaves and Water Samples by Magnetic Dispersive Solid Phase Extraction Based on β-Cyclodextrin Functionalized Graphene Oxide Followed By GC-FID

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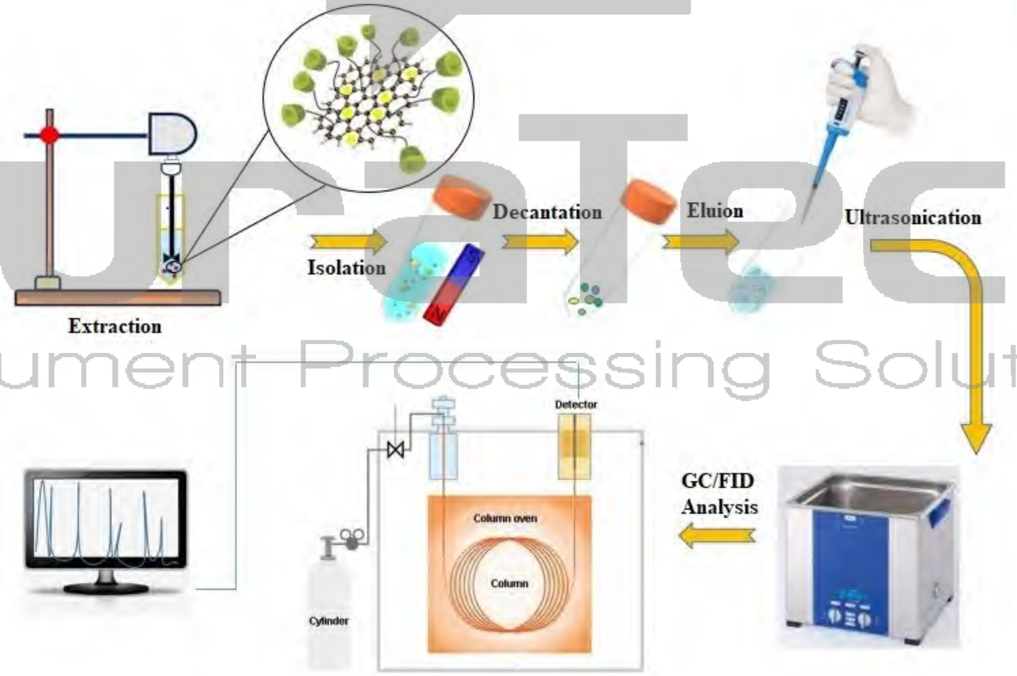
Graphical Abstract



Abstract: A high-performance sorbent was synthesized and used to extract some polycyclic aromatic hydrocarbons (PAHs), (naphthalene, acenaphthene, fluorene, phenanthrene, fluoranthene, pyrene, benzo[a]pyrene) from environmental samples by using magnetic dispersive solid-phase extraction (MdSPE) procedure followed by GC-FID. The sorbent was synthesized by grafting β-cyclodextrin (CD) onto magnetic graphene oxide (MGO) via hexamethylene diisocyanate (HMDI) as a crosslinker. Good reusability, high surface area, and high PF values and fast extraction kinetics are the advantages of the introduced sorbent. Materials which originated from the nature such as dextrins, have attracted wide attention due to their excellent properties such as biocompatibility, low-cost, nonimmonogenic, chemical inertness and so on. Prepared magnetic sorbent (MGO/HMDI/β-CD) was characterized by Fourier transform infrared spectroscopy (FTIR), the field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), the X-ray diffraction (XRD), vibrating-sample magnetometer (VSM), and energy-dispersive X-ray spectroscopy. The variables that affect the performance of the extraction method were investigated in detail, and thoroughly optimized using experimental design and response surface methodology. Under the optimum conditions (sorbent amount: 25 mg, extraction time: 20 min, concentration of NaCl: 27% (w/v), desorption time: 6 min, volume of desorption solvent: 300 µL, and desorption solvent: toluene) preconcentration factors were obtained between 46 and 62. The results indicated that the extraction recoveries of these compounds were in the range of 73.0-97.1%. Good linearity within the range of 5.0-1000.0 ng/mL with coefficients of determination higher than 0.984 were achieved. Detection limits were found to be 0.1-0.5 ng/mL, while the relative standard deviations (RSDs) were calculated to be ≤ 8% (n = 3). The fabricated sorbent was successfully applied for the extraction and quantification of PAHs in pretreated environmental samples (soil, tree leaves, and river water).

Keyword: β-Cyclodextrin; Environmental samples; Hexamethylene diisocyanate; Magnetic dispersive solid phase extraction; Polycyclic aromatic hydrocarbons

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Environmentally Friendly and Selective Oxidation of Sulfides and Oxidative Coupling of Mercaptans in The Presence of Fabricated Oxo-Vanadium on Modified MCM-41 with 5-Nitro-2-Hydroxy Benzaldehyde

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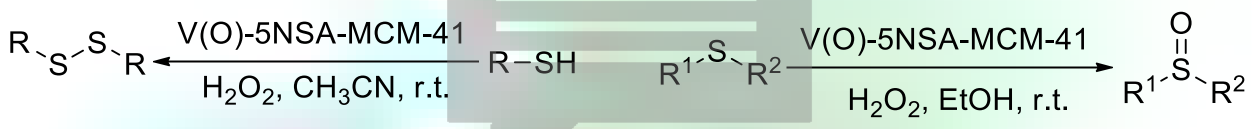
Graphical Abstract



Abstract: In recent years, nanomaterials have been widely used as solid supports for the immobilization of homogeneous catalysts. Among the various nanomaterial, MCM-41 has high stability, and large specific surface area. High thermal stability of MCM-41 allows the application of MCM-41 in harsh condition and its heterogeneity nature allows the recycling of supported catalysts. Also, the large pore volume of MCM-41 allows supporting of metal complexes into its channels. Therefore, we are reporting a Schiff-base ligand of 5-nitro-2-hydroxy benzaldehyde on MCM-41 for fabrication of oxo-vanadium (V(O)-5NSA-MCM-41) as an environmentally friendly, efficient and reusable catalyst for the selective oxidation of sulfides and oxidative coupling of mercaptans. Because, oxidation reactions are one of the powerful tools and practical methods for the synthesis of biologically actives compounds and transformation of organic functional groups. For example, they have some of biologically active such as antiulcer, antibacterial, antifungal, anti-atherosclerotic and anti-hypertensive. In this work, H_2O_2 was used as environmentally friendly oxidant reagent. Because among the various oxidants such as metal oxidants, organic oxidant, peroxides and halogens, H_2O_2 is an available, inexpensive and environmentally benign oxidant.

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Adsorptive Stripping Square Wave Voltammetric Determination of Oxycodone by an Overoxidized Poly(4-aminophenol) Modified Glassy Carbon Electrode

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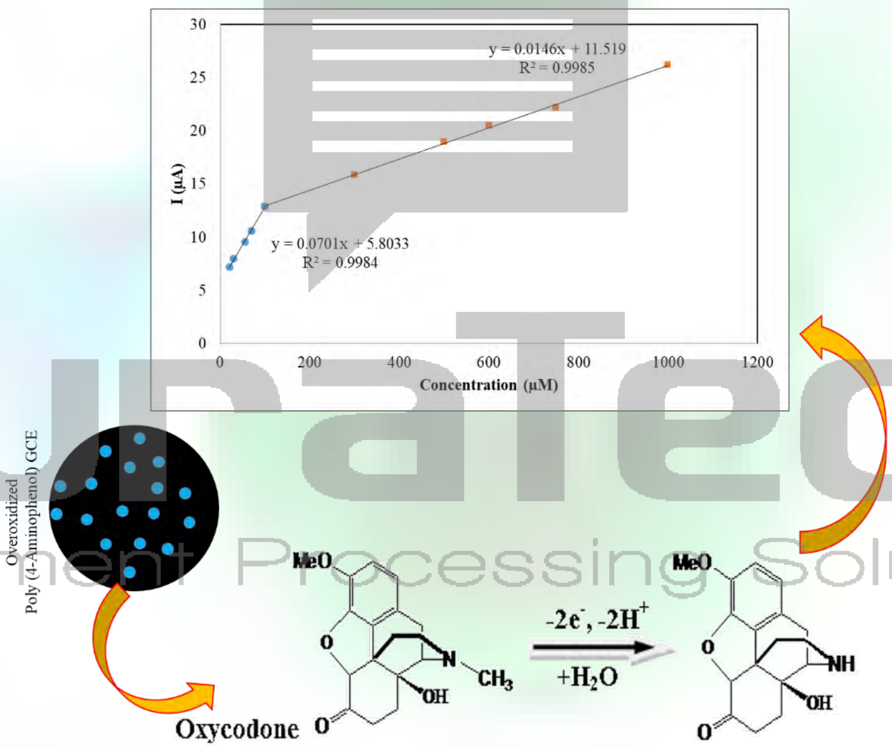
Graphical Abstract



Abstract: Oxycodone is an opioid medicine that is widely prescribed for the treatment of the diseases that are accompanied with sever and chronic pains. In the recent decade, residual pharmaceutical compounds (especially antibiotics and analgesics) have begun to be considered as emerging environmental pollutants due to their continuous input and persistence to aquatic ecosystem even at trace concentrations. Besides, oxycodone is very addictive and at high dosages cause serious life-threatening side effects including bradycardia, circulatory collapse, respiratory depression and even death. In this respect, developing a rapid, simple and sensitive analytical method for the determination of oxycodone is very important. Therefore, in this study, overoxidized poly(4-aminophenol) was electrosynthesized on the surface of a glassy carbon electrode and its applicability for the measurement of oxycodone was investigated for the first time. The modified electrode was characterized by Fourier-transform infrared spectroscopy (FT-IR), cyclic voltammetry (CV) and square wave voltammetry (SWV) techniques. The obtained voltammograms showed a well-defined peak for oxycodone at +1.36 V (vs SCE). The influence of all of the effective experimental parameters on the signal intensity was investigated and optimized. Under the optimized conditions, the designed sensor exhibited two dynamic ranges (20-100 μM) and (100-1000 μM) with $y = 0.0701x + 5.8033$ ($R^2=0.9984$) and $0.0146x + 11.519$ ($R^2=0.9985$) equations respectively. The values of limit of detection (LOD) and limit of quantification (LOQ) were 5.75 and 19.17 μM respectively.

Keywords: Oxycodone, Adsorptive stripping square wave voltammetry, Poly(4-aminophenol), Electrochemical sensor.

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Electrochemical Determination of Acetaminophen by a Glassy Carbon Electrode Modified with Over-Oxidized Poly 4-Aminophenol

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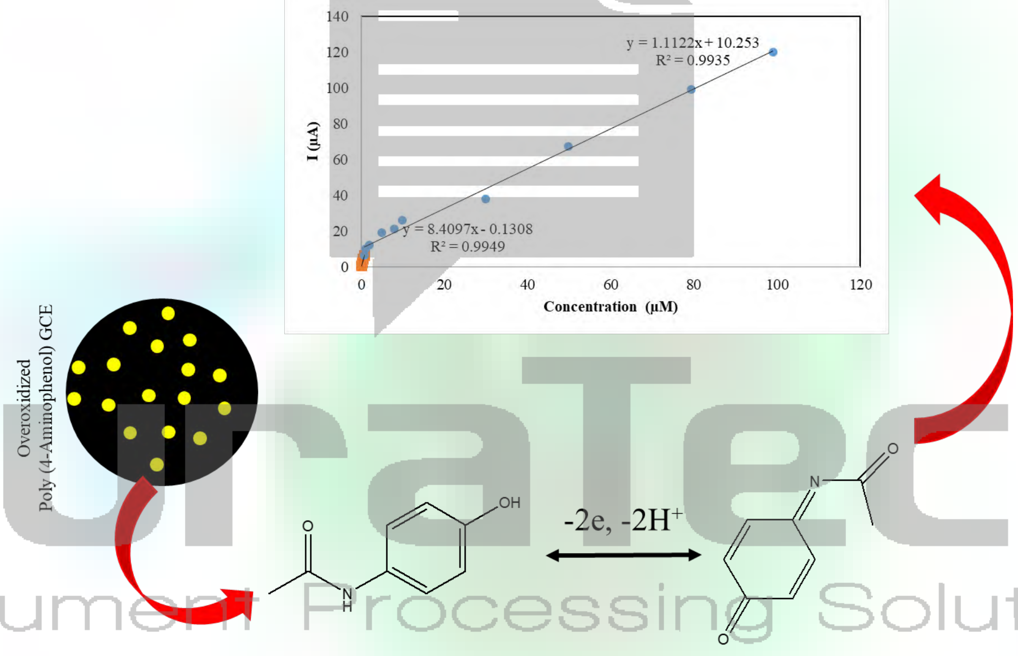
Graphical Abstract



Abstract: Contamination of the environment is an important issue that can influence the human being health and the life quality. One of the new emerging contaminants s is acetaminophen, that is widely used as a painkiller, analgesic, and antipyretic medicine globally. It was reported that 58–68% of acetaminophen is excreted by human urine and it is also prone to bioaccumulation in aquatic organisms. In this regard, a novel electrochemical sensor based on over-oxidized poly 4-aminophenol was fabricated for determination of trace amounts of acetaminophen. 4-aminophenol

was polymerized electrochemically on the surface of glassy carbon electrode (GCE) by cyclic voltammetry method and then overoxidized by applying constant potential (+1.2 V (vs SCE)) in order to increase its conductivity, porosity and electrocatalytic activity. Subsequently, the modified GCE was employed for anodic stripping square wave voltammetric determination of acetaminophen. Square wave voltammograms of acetaminophen solutions using the modified GCE showed a well-defined peak at +0.63 V (vs SCE). In order to achieve the highest sensitivity, all of the operational and instrumental parameters including pH, nature of supporting electrolyte, accumulation time, accumulation potential, frequency, pulse amplitude and voltage step were optimized. The results showed that the maximum peak current with normal shape could be obtained at pH=2, KNO3 0.1 M (as the supporting electrolyte), 60 S (accumulation time), 0.055 V (accumulation potential), 75 Hz (frequency), 50 mV (pulse amplitude) and 10 mV (voltage step). Under the optimum conditions, the proposed sensor showed a wide linear range over the concentration range of 0.3-100 µM with a correlation coefficient of 0.9949. The reproducibility of the designed sensor was also evaluated for five replications (10 µM solution of acetaminophen) and the %RSD value was and %3.2. The limit of detection (LOD) and limit of quantitation (LOQ) values of the developed sensor were 0.07 µM and 0.23 µM respectively.

Keywords: Acetaminophen, Square wave voltammetry, Glassy carbon electrode, Electrochemical sensor.

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5-Nitro-Salicylaldehyde Schiff-Base Complex of Cobalt on MCM-41 as an Environmentally Friendly and Selective Nanocatalyst for The Synthesis of Sulfoxide Derivatives

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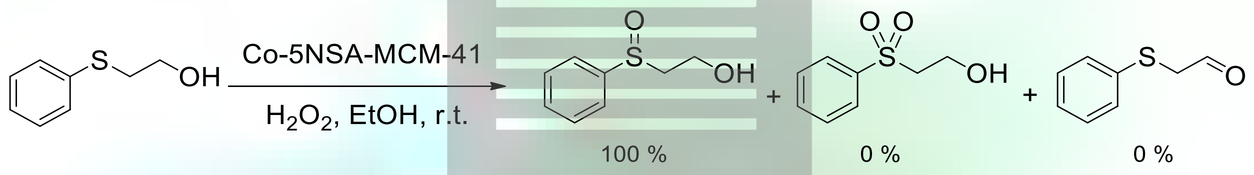
Graphical Abstract



Abstract: The selective oxidation of sulfides to sulfoxides is an interest procedure in organic synthesis, because sulfoxides play an important role in enzymes activation, separation of radioactive or less common metals and in medicinal chemistry as antibacterial, antihypertensive, antifungal, anti-atherosclerotic agents, anti-ulcer, and cardiotonic agents. However, the synthesis of sulfoxides from sulfides have been widely reported by both organic and inorganic oxidant reagents, which lead to toxic wastes and byproducts. Therefore, to keep pace green chemistry principles, herein we have used hydrogen peroxide as an environmentally friendly oxidant in the synthesis of sulfoxides from sulfides using H_2O_2 in the presence of Co-5NSA-MCM-41 as selective, reusable, stable and environmentally friendly catalyst. Because, use of H_2O_2 as oxidant offers several advantages such as cheapness, readily available, and environmentally friendly oxidant with the water as only byproduct. Also, ethanol is also used as a solvent, which is completely environmentally friendly because it is cheap, available and non-toxic.

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Adsorption of Methylene Blue onto Nanosized Transition Metal Spinels with High Surface Areas from Zeolite Y: Adsorption Isotherms, Kinetic and Thermodynamic Studies

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Graphical Abstract

Abstract: Spinel particles with sizes in the nanometer range having high surface areas are obtained by the calcination of transition metal exchanged zeolites. The spinel crystallites grow within an amorphous silica matrix, formed by the collapse of the zeolite framework. Dissolution of this matrix leads to the high surface area spinels. The compositions of the zeolites, as well as the calcination conditions, have an influence on the type of phases formed and on the properties of the phases. The adjustment of these conditions enables control of the size of the spinel particles. Removing dye pollutants from industrial waste water is a common environmental application of nanomaterials. This study investigated in-situ synthesis and adsorbing ability of a Nano Catalyst Mixoxides - Zeolite- for Methylene Blue (MB) dye. To determine composite structure, chemical bonds ,morphological features X-ray diffraction (XRD), Fourier transform of infrared

spectroscopy)FTIR) and Field Emission Scanning Electron Microscopy (FESEM) were examined and adsorbent capacity (function of solution pH, time of removal and material content) for Methylene Blue (MB), by four method (Isotherm Langmuir, Redlich–Petersonand, Linear regression and Isotherm Freundlich) were studied. Experimental results of Mixoxides -Zeolite-nanocomposite showed average removal adsorbent of 70% in 30 minutes and removing by external magnetic field in a minute. This study shows that the synthesized nanocomposite advances for high amount of pollutant cleaning in a short time by using small amount of materials.

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A DFT Study on The Host/Guest Inclusion Process of Sarin into β-Cyclodextrin

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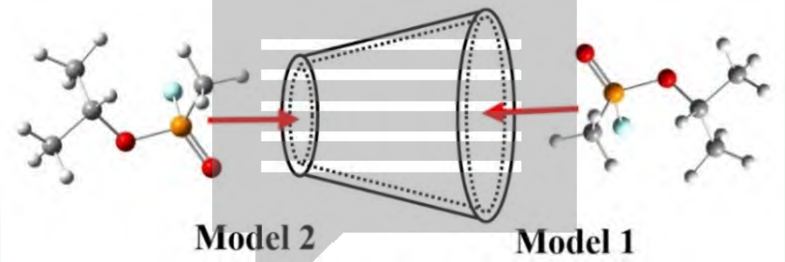
Graphical Abstract



Abstract: Herein, it has been described a study on the inclusion complex formation and molecular interactions between nerve agent sarin and scavenger β-cyclodextrin (β-CD) by performing quantum mechanical calculations including PM6 semi-empirical and density functional theory (DFT) in vacuum and in water. Two models (model 1 and model 2) of complexation were taken into consideration. First, the docking process was investigated between sarin and β-CD using the PM6 method to find the most stable structure. Next, the energy decomposition, the global reactivity descriptors, and finally, natural bond orbital (NBO) calculations on the most stable complex were continued with the DFT computations. The obtained results clearly indicated that the formed complexes are energetically favored with or without solvent. Analysis of the electronic chemical potential as a reactivity descriptor showed that the encapsulation process is spontaneous. The NBO calculations confirmed the existence of hydrogen bonding between sarin and β-CD in both vacuum and water.

Keywords: Sarin, β-Cyclodextrin, Inclusion complex, DFT

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Studies on the Extraction of Chitin from the Shell of Different Species of Bushehr Sea Shrimp and Its Application in Removal Methylene Blue Dye in Wastewater

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Graphical Abstract

Abstract: Marine organisms such as shrimp, crabs, krill, and squid contain the natural polymer chitin. Chitin can be defined as a natural macromolecule as well as the most abundant and second natural polysaccharide produced by living organisms after cellulose. Chitin has many applications in the field of chemistry and medicine, including the production of antibacterial and antifungal drugs, contraceptives, synthesis of chitosan through deacetylation of chitin, absorption of heavy metals, etc. Shrimp skin is abundant in local markets in southern Iran, including Bushehr, which contains valuable compounds such as chitin, amino acids, pigments and fatty acids. Because half

or more of the shrimp is considered as skin and discarded, eventually several thousand tons of shrimp skin is discarded annually, so in addition to environmental problems, it leads to a waste of capital. Removal of minerals, organic matter, and pigments from shrimp skin leads to chitin synthesis. [1-5]

In recent decades, among industrial wastewaters, the study of the decolorization and degradation of pollutants from paint effluents has received much attention. The production of synthetic dyes and widespread use of these dyes in various industries such as textile, plastic, paper, fabric, and cosmetics has led to the production of dye wastewater. Hence, this is considered a dangerous environmental warning and a major source of water pollution. It is worth mentioning that, water is an important resource in the ecosystem as well as the survival of human life. Unfortunately, in recent decades, due to a large amount of water used in the dyeing industry, this pollution can be considered as one of the largest and most important pollutants in liquid wastewater. Hence, several methods were used, including chemical, physical, and biological methods, to remove wastewater from dyes or convert them into low-risk by-products. Generally, dyes can be divided into two categories: ionic dyes and non-ionic dyes. Non-ionic dyes can be divided into diffuse dyes and in addition, ionic dyes can be divided into two categories: cationic dyes(base) and anionic dyes (direct; acidic; reactive). The most important and well-known cationic dye is methylene blue. [6-8]

The aim of this study was to extract chitin from the shell of different species of Bushehr marine shrimp and also its application in removing methylene blue dye in wastewater through the use of living marine resources and also overcoming environmental problems.

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The Role of Environmental Education in the Management of Protected Areas (Case Study: Sorkhabad Protected Area in Zanjan Province)

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Abstract: This study aimed to investigate the role of local communities' education in the management of Sorkhabad protected area in Zanjan province. Sorkhabad protected area with an area of 119225 hectares is one of the protected areas under the management of the Environmental Protection Organization in Zanjan province, which includes habitat of species such as: deer, leopard, wild cat, brown bear, boar, hyena, wolf, squirrel, peacock and etc. This research uses a variety of tools such as library studies (reviewing books, magazines, related articles, internet search, etc.), interviewing local community residents and environmentalists, two questionnaires for local community residents and experts (university professors, experts, and experts). A questionnaire was developed to conduct this research. The statistical population of this study is 23843 people living in cities and villages of Sorkhabad Protected Area. The sample size is 387 people which is obtained using Cochran's formula. The validity of the questionnaires was confirmed by 5 experts and the reliability of the questionnaire of local community residents with 45 questions with 5 Likert scale options was equal to 0.915 and the questionnaire of experts by 12 university professors, experts and senior environmental experts in the template of 102 standard AHP questions was completed by pairwise comparison. AHP (Analytical Hierarchy Process) model and Expert Choice and SPSS softwares were used to analyze the questionnaires. The findings of this study showed that the role of education of local communities in the management of Sorkhabad protected area is significant. The people of the region do not have enough knowledge about protected areas, the importance of biodiversity, the duties of the Environmental Protection Organization, the role of education in environmental protection, etc. So it is necessary to pay serious attention to environmental education in protected areas. The findings also showed that people's environmental knowledge has a great impact on their environmental attitudes and behavior.

Keywords: environment, wildlife, local communities, habitat, environmental education, participation, biodiversity.

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Investigation of Land Use Changes Around Glabar Dam in Ijroud-Zanjan City Under The Influence of Dam Construction

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Abstract: Land use change is one of the most important and fundamental manifestations of environmental change caused by human activities. Construction of dams is one of the most important and fundamental human drivers of land use change. The main purpose of this study was to investigate the impact of construction of the Golabar Dam on the use of upstream and downstream flood events in the Golabar catchment. In this regard, Landsat satellite images were used for two years 2011 and 2018, before the Glabar Dam was flooded and 7 years after the dam was exploited. The 2011 satellite images were obtained from Landsat TM TM sensor and 2018 from Landsat 8 OLI / TIRS satellite from Earth Explorer database. Pre-processing of images was performed in ENVI and ARC-GIS software. To detect land-use changes, MLH supervised classification algorithms were used, using a number of field sampling. After detecting land use changes during the two periods of 2011 and 2018, the T-Student test of confidence level of 0.95 was used. The results indicated that in total 7 land use classes or main land cover were extractable in Golabar basin, including gardens, dryland, irrigated agricultural lands, residential towns and villages, poor rangelands, medium rangelands, and meadows. Blue. The results of the analysis of land use changes in the two periods before and after dam dam showed that changes occurred in all revealed land uses during the study period. Both land use and land cover of the poor rangelands and the average rangelands both experienced a decreasing trend during the period 2011 to 2018. While irrigated agricultural land use has increased and land use related to dryland agriculture has not changed significantly during the period under review. During the 7-year period under review, the land use increased by 2583 hectares, accounting for about 3% of the total area of dryland

agricultural land in 2011. Garden areas have more than doubled over the period under review, with the 2018 area increasing by 2.7 times as compared to 2011. Residential areas comprising urban and rural areas in the study area have almost doubled over the seven-year statistical period from 2011 to 2018. So that the area of this land use increased over the 7-year period of 19672 hectares. Statistical analysis using two-way parametric T-student test showed that there were not enough changes in the level of confidence to be considered significant. Therefore, during the last 7 years, from 2011 to 2018, the reported user changes were generally not significant enough to be significant at the confidence level of 0.95.

Keywords: Land use, Dam construction, Gulabar basin, supervised classification.

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Photocatalytic Degradation of Methylene Blue by CeO_2 Nanoparticles

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Abstract: Over the last decades, the removal of wastewater using active photocatalytic systems has attracted considerable attention, which has led to the development of various nanostructured catalysts for treatment of wastewater. In this regard, the role of pollution of toxic and non-degradable organic dyes that leave their destructive effects on the environment for a long time is undeniable. These compounds are widely used in the textile, leather, paper, food, plastic and cosmetic industries. Methylene blue dye is a multi-nuclear aromatic compound that can not only cause acute toxic effects, but also cause some serious problems such as shortness of breath, chest pain, dizziness, syndrome, burning sensation, nausea, vomiting and diarrhea. In this project, the CeO_2 nanoparticles were prepared using simple Co-precipitation method. Synthesized CeO_2 nanoparticles were characterized by XRD, FESEM & DRS technique. The effect of key parameters such as initial pH, photocatalyst dosage, initial dye concentration and irradiation time on dye removal efficiency were studied. The results of dye removal show that the initial dye concentration has no effect on the removal percentage, but by increasing the pH of solution, the amount of dye removal was increased, and the maximum efficiency was achieved at pH=8. Also, by increasing the photocatalyst dosage from 0.01 to 0.05 mg/100mL and increasing the irradiation time from 10 to 30 minutes, the color removal efficiency was increased. Maximum photocatalytic degradation of Methylene Blue was about 71.76% at pH=3, 30 mg/L of initial Methylene Blue concentration, 0.05 mg/100mL of CeO_2 nanoparticles at 30 min of irradiation time. However, the results indicated that the photocatalytic degradation of Methylene Blue best fitted with pseudo-first order kinetic model. According to the experiments, the CeO_2 nanoparticles has high potential for removal of Methylene Blue under UV light (300 watt).

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EDTA Functionalized Ordered SBA-15 Mesoporous Silica as an Effective Adsorbent for Preconcentration of Some Heavy Metal Ions Followed by ICP-AES

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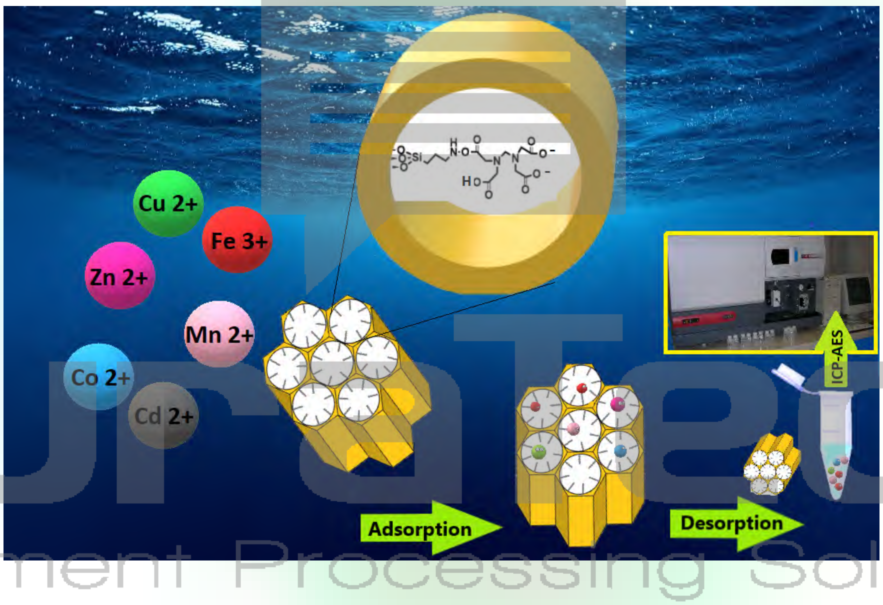
Graphical Abstract



Abstract: Heavy metal ions create serious environmental and public concerns at a global scale. Inductively coupled plasma atomic emission spectrometry (ICP-AES) has been reported for determination of metal ions. For determination of trace metal ions in complicated environmental samples, the direct analysis of them by analytical instruments is usually difficult. Therefore, sample pretreatment is necessary and unavoidable.

The large pore size (2-50 nm) of mesoporous silica adsorbents provides high specific surface area for the uptake of pollutants from water samples. The coordination sites of ethylenediaminetetraacetate (EDTA) include two amines and three carboxylate groups, which can be occupied with heavy metal ions to form a stable (1:1) complex.

The aim of this work was to develop a simple, efficient, and sensitive method to extract and preconcentrate Co^{2+}, Mn^{2+}, Cu^{2+}, Zn^{2+}, Fe^{3+}, and Cd^{2+} with EDTA functionalized ordered mesoporous silica (EDTA-SBA-15) as a potential adsorbent. The extracted ions were eluted and analyzed by the flow injection ICP-AES.

The effect of analytical parameters, such as the sample pH, amounts of the adsorbent, adsorption and desorption times, sample volume, eluent type, eluent volume on the extraction efficiency of the metal ions were investigate. Under optimized conditions, the limits of detection of Co^{2+}, Mn^{2+}, Cu^{2+}, Cd^{2+}, Zn^{2+}, and Fe^{3+} were found to be 50, 5, 10, 50, 10, and 500 ng L^{-1}, and the relative standard deviations for determination of 50 µg L^{-1} were 5.3, 5.3, 4.6, 1.7, 4.4, and 5.78% (n = 4), respectively. Linear ranges were obtained for the selected metal ions including Co^{2+}, Cu^{2+}, Cd^{2+}, Zn^{2+} (0.1-250 µg L^{-1}), Fe^{3+} (1-250 µg L^{-1}), and Mn^{2+} (0.01-25 and 50-500 µg L^{-1}) with perfect correlation coefficients (R = 0.9958-0.9996, n = 8). The applicability of the introduced adsorbent was evaluated by the extraction and determination of the heavy metal ions in different environmental water samples.

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Pollution Indices of Heavy Metals (Zn, Cu, Cd, Pb, Ni and Fe) in Surface Soils of Zanjan Province

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Abstract: Due to increasing the heavy metal pollution and its related diseases in society [1-2], distribution analysis and calculation of the health risk of this pollution in the human environment are very important. Therefore in the present study, the concentration levels of heavy metals such as Zn, Cu, Cd, Pb, Ni and Fe in soil samples collected from 357 sampling locations around Zanjan Province, Iran were analyzed. To interpret and to evaluate the pollution status and distribution of heavy metals in soil, metal pollution parameters such as enrichment factor (EF), geoaccumulation index (Igeo), pollution factor (CF), potential ecological risk index (RI) and pollution Load index (PLI) and geospatial distribution patterns were used. Results indicated that the mean concentrations of Cd and Pb exceeded the world crustal average. Statistical analysis results showed that Zn, Cd and Pb levels in the investigated region were highly influenced by anthropogenic inputs such as metal extraction and mining activities. According to the health risk assessment model introduced by USEPA to evaluate the human health risks, the none-carcinogenic risk for children was above adults. Total potential carcinogenic health risks for both children above the threshold level and for adults in the study area were in acceptable range.

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Investigation of Rhodamine B Adsorption by using ZnS/montmorillonite/g-C_3N_4

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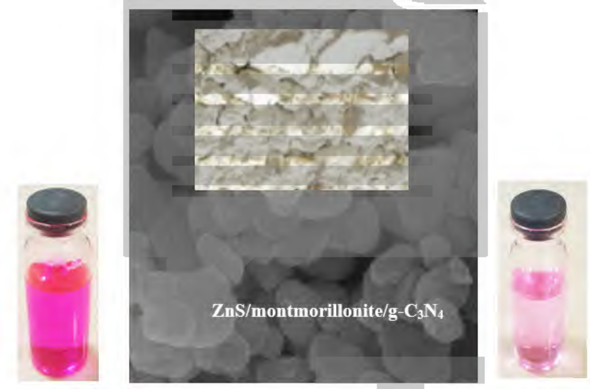
Graphical Abstract



Abstract: The water pollution become an important subject, because of the release of manufacturing effluents. Physical, chemical, and biological strategies are employed to the decrease of pollutant, which the adsorption is well-known as a benefit method. It is of great significance the design of novel composite with high yeild. Graphitic carbon nitrides (g-C_3N_4) as an organic polymer have attracted researchers in many fields. In this regard, the ZnS/montmorillonite/g-C_3N_4 was synthesized by a simple route to improve g-C_3N_4 property, and the synthesis was confirmed by Fourier transformed infrared (FIR), Scanning Electron Microscopy (SEM), and X-ray Diffractometer (XRD) analysis. The Rhodamine B (Rh. B) removal was studied through RSM-CCD design, and the influence of parameters was considered via 50 runs. Based on the obtained data, the as-synthesized composite can be applied for the Rh. B removal with high yield.

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Application of Medlar Core Powder to Remove Methylene Blue from Aqueous Solution

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Abstract: The efficiency of medlar core powder as a low-cost adsorbent for removing a cationic dye methylene blue (MB) from aqueous solution has been investigated by using batch mode and continuous systems experiments. The effects of different parameters namely amount of adsorbent, initial dye concentration, contact time, temperature and pH solution of dye solution have been studied to understand the adsorption behavior of the adsorbent under various conditions. Various techniques for characterizing the adsorbent have been applied including, zero point charge measurement (pHpzc), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). The experimental isotherm data have been analyzed using Langmuir and Freundlich isotherm equation. Methylene blue adsorption fitted the Langmuir isotherm. The kinetic results of adsorption obeyed a pseudo-second order model. Thermodynamic parameters including the Gibbs free energy ΔG°, enthalpy ΔH° and entropy ΔS° have revealed that the adsorption of methylene blue on the medlar core powder is feasible, spontaneous and endothermic. The maximum removal percent 25mL of methylene blue solution is 96.4% for 100 mg/L of MB under conditions, pH=7 at a temperature 25 °C and 0.08 g/L of adsorbent.

Keywords: Medlar core powder, Methylene blue, adsorption, Langmuir adsorption isotherm, kinetic of adsorption

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A Nanozyme-Based Sensor for Colorimetric Detection of Tacrolimus by Using UiO-66-NH$_2$ Metal Organic Framework

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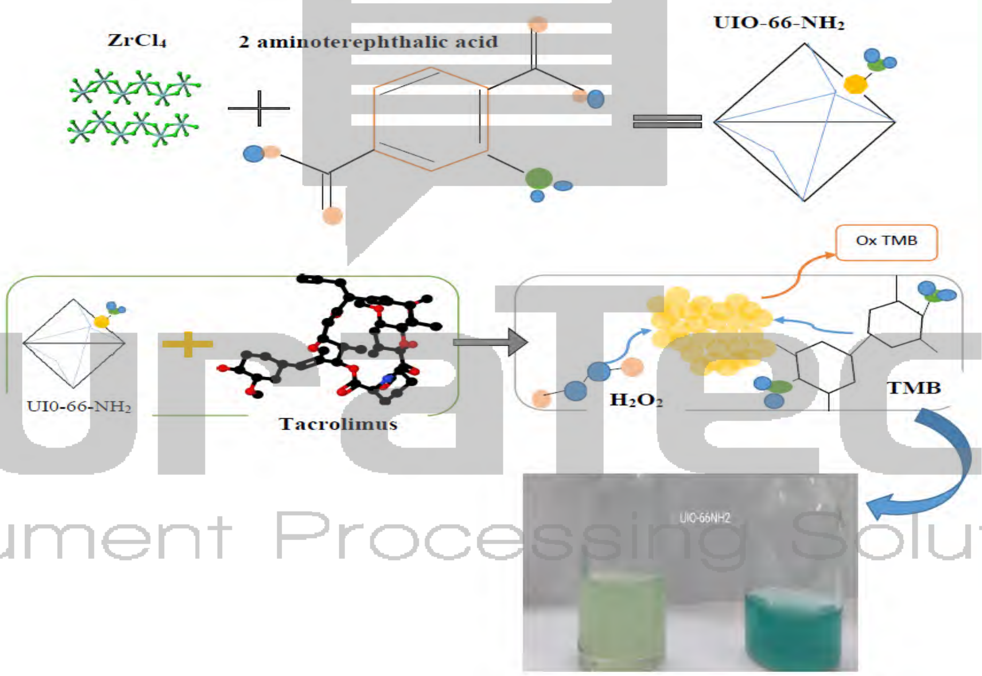
Graphical Abstract



Abstract: A aunctionalized Zr based metal-organic framework (MOF) nanoparticles were synthesized using a one-step solvothermal method. The as-prepared UiO-66-NH$_2$ nanoparticles acting as nanozymes, have been developed for highly sensitive and selective detection of tacrolimus with the substrate 3, 3′, 5, 5′-tetramethylbenzidine (TMB) within a few seconds in the presence of hydrogen peroxide (H_2O_2)[1]. The synthesized MOF was characterized by powder X-

ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FT-IR). The XRD pattern of UiO-66-NH_2 was consistent with the reported results of UiO-66 which confirms crystallinity structure and suitable formation of the functionalized particles. The results of TEM and SEM showed that the particles are in spherical shape with the average size of 100-150 nm. It was also revealed that UiO-66-NH_2 crystals were inter-grown. FTIR spectra of the solution after sensing illustrated two new peaks which corresponds to proper interactions between the medicine and the nanosensors. These interactions were also affects the size of the tacrolimus particles to increase after sensing. Changing the color of the solution directly from yellow to blue confirms that the nanosensors are able to oxidize TMB to blue color oxidized TMB (oxTMB). Optimum concentration of both TMB and H_2O_2 were experimentally found to be 30mM. The maximum peak wavelength of oxTMB was observed at 650 nm[2]. The addition of tacrolimus and then increasing its concentration led to the production of different products in blue color. A comparison has been done on the sensing of UiO-66 and UiO-66-NH_2 which proved that the functional MOF can speed up the sensing. In experimental measurements, the limit of detection was obtained 0.5 mg/L. It can be concluded that the simple and sensitive UiO-66-NH_2/TMB/H_2O_2 colorimetric system can have great promising applications in clinical medicine.

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A Review on Ceramic Membrane

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Abstract: The use of membrane technology in various processes of processing materials is increasing and the use of this technology in the water and sewage industry is also expanding. Ceramic membranes are one of the types of membranes used in recent years in the field of water and wastewater. These membranes can be replaced by micron filters because of their physical structure and pore size. These membranes have more thermal resistance and also corrosion resistant. Ceramic membranes are made by combining metals such as aluminum, titanium, calcium and ... with a non-metal in the form of nitrite or carbide oxide. Ceramic membranes made from such materials are the most important group of inorganic membranes. Aluminum oxide and zirconium oxide are among the most important materials in this group. The porous ceramic membrane configuration is mainly composed of three types: flat sheet, tube type and multi-channel, and plastic membrane is mainly used for small industrial production and laboratory research. The membrane is combined to form a tube heat exchanger, which can increase the membrane filling. However, due to the power problem, industrial applications have disappeared. The ceramic membrane of the scale program usually adopts a multichannel configuration setting, that is, several channels are distributed in a circular section, and the number of public channels is 7, 19, 37, and so on[1]. The main methods for producing ceramic membranes include preparation of solid particles, carrier membranes and microfiltration, ultrafiltration membranes and nanofiltration, using a glass membrane made from a divided phase, using a special technology (such as chemical vapor deposition and electrolysis coating, etc.) [2].

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The modified removal of benzothiophene using Ni-NaY Zeolite Adsorbent System

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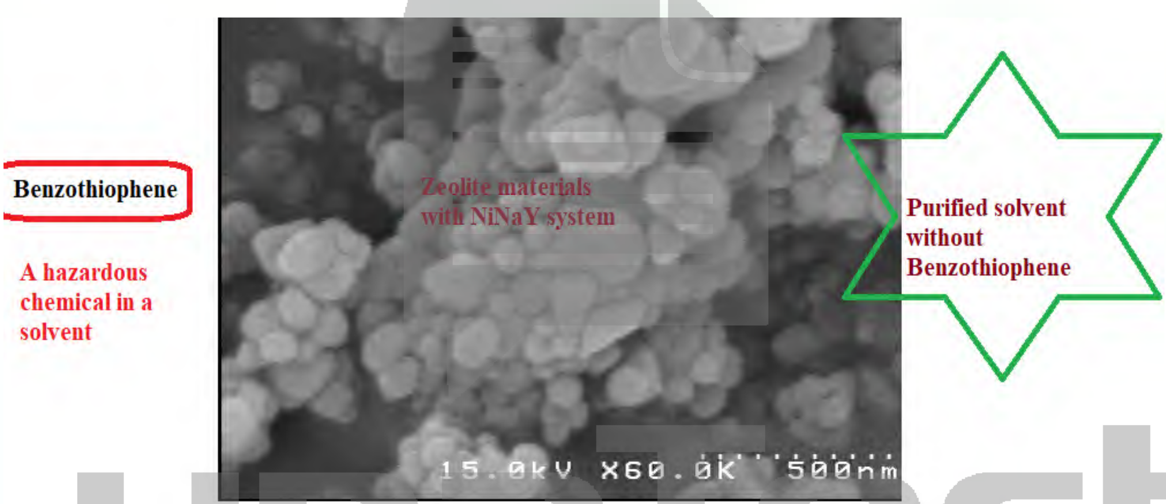
Graphical Abstract



Abstract: The present work was designed to synthesize novel NiNaY zeolite systems for efficient adsorption of benzothiophene. The Ni-NaY was prepared by ion-exchange method. The characterization of Ni-NaY was done by EDX, FTIR, TGA, BET, SEM, and XRD. Characterization results revealed that Ni-NaY showed an increased surface area and pore volume compared to NaY. The adsorption experiments show that the desulfurization performance of NiNaY decreases up to 99%. FT-IR spectra of benzothiophene adsorption indicate that benzothiophene is mainly adsorbed on NiNaY via π electron interaction. The gas chromatography analysis (GC) was used for the calculation of the organic matter concentrations. The effect of various parameters such as adsorbent dosage, temperature and pH on the adsorption was investigated.

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Efficient Oxidation of Symmetrical Sulfides to Sulfoxides Over Ni Modified NaY Zeolite

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Abstract: Ni modified NaY zeolite was prepared and investigated for their potential for the selective oxidation of symmetrical disulfides containing aromatic and aliphatic sulfides and thiols with molecular oxygen as the sole oxidant. The solid catalyst has been identified using TGA, FT-IR, SEM, and XRD. The XRD pattern of Ni modified NaY zeolite shows a cubic phase of crystal system with the Fd-3m space group. The as prepared catalyst has high surface area as determined by BET method. Various derivatives of aromatic sulfides with the electron-donating and electron-withdrawing substituents on the aromatic ring have been investigated. The reported procedure is fast, simple and the yields are excellent (>90%) in most cases with low reaction times. Moreover, Ni modified NaY zeolite as a catalyst can also be separated and recycled several times without any remarkable decrease in its catalyst activity. In comparison, aromatic sulfides have higher yields than those of aliphatic ones.

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Differential Pulse Electrodeposition of Vanadium Pentoxide Nanostructures for High Performance Polymer Solar Cells

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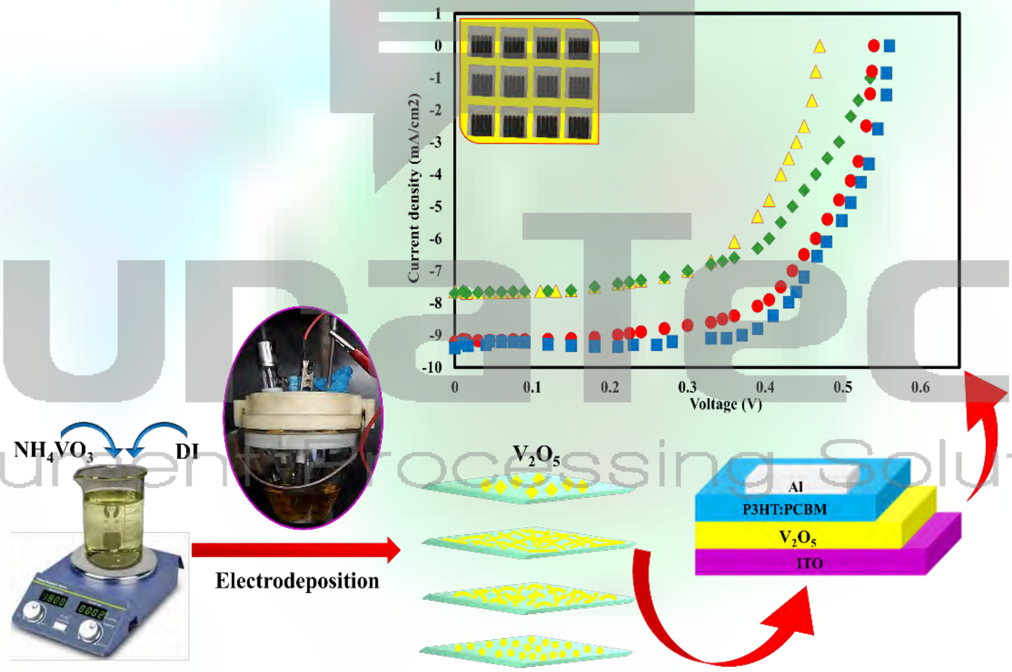
Graphical Abstract



Abstract: Solar energy, with features like interminable is the most promising technology to solve the energy crisis. In recent years, 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 and compatibility with flexible substrates [1]. BHJ PSCs consist of three main substrates: anode, photoactive layer and cathode. The other two components which improve the PSCs' performance are the electron transport layer and the hole transport layer (HTL) .The HTL task is to improve the anode's efficiency in collecting the holes in PSCs. The HTL should have good stability, high electrical conductivity, low resistance and high working function .For current PSCs with indium tin oxide (ITO) as the anode, PEDOT:PSS has been widely used as the HTL due to its high work function and smoothing out the rough ITO .Unfortunately, the strong acidity of PEDOT: PSS causes problems such as degradation of cell stability [2]. VO_x is a promising candidate due to its relatively high charge transfer mobility and environmental stability .Vanadium Pentoxide (V_2O_5) has special applications in different fields, such as optical detectors, light-converting devices, lithium-ion batteries and solar cells .V_2O_5 can be synthesized using different methods such as hydrothermal, sol-gel and electrodeposition [3, 4]. In this work, V_2O_5 nanostructures were grown on the ITO-coated glass slides using differential pulse voltammetry (DPV) method and utilized as the interfacial layer in the construction of BHJ PSCs. The influences of deposition time and applied potential were investigated. Simple adjustment of the applied potential regime and deposition time led to considerable structural and electrochemical changes of the resulting V_2O_5. Features of the electrochemically-grown V_2O_5 were compared with each other. The best sample was selected in terms of suitable surface conductivity, high optical transparency and appropriate energy levels and applied as HTL in BHJ PSCs. Results revealed that the optimum V_2O_5 sample provided considerably better electrical, optical and electrochemical features. V_2O_5 nanoparticles synthesized with DPV, showed the high electroactive surface area (0.26 cm^2), high charge mobility ($2.44\times10\text{-}4\ cm^2.V^{-1}s^{-1}$) and excellent conductivity (0.03 $mS.cm^{-1}$). The best cell provided an open circuit voltage of about 0.56 V, a short circuit current of 9.42 mA cm^2, a fill factor of 65.3% and a PCE of 3.40%. PCE of this cell was about 60% higher than that considered for the reference device prepared base on the PEDOT:PSS HTL.

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Detection and Determination of Mercury and Glutathione Based on the On-Off Fluorescence of Functionalized Metal-Organic-Framework as Nanosensor

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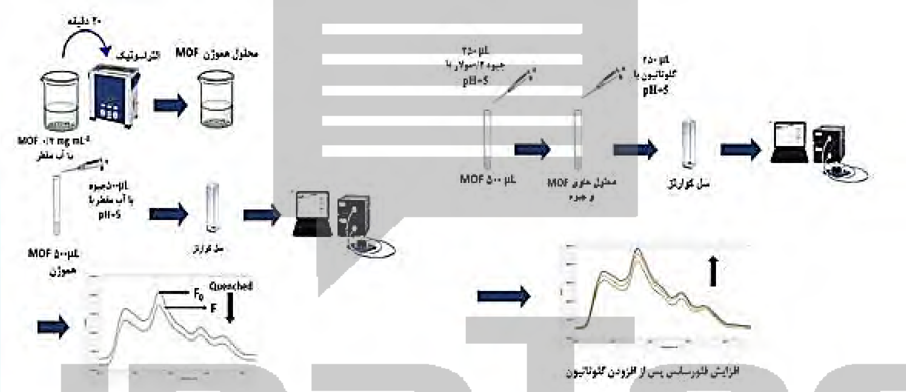
Graphical Abstract



Abstract: Metal-organic frameworks, called coordination polymers, are composed of building blocks such as organic ligands and metal ions that are joined by coordination bonds [1]. The sensitive luminescence properties of MOFs have led to the development of sensor applications of LMOFs [2]. In this study, a simple, selective, and sensitive fluorescence sensor based on the functionalized metal-organic-framework was designed for the detection and measurement of Hg^{2+} and glutathione. The addition of Hg^{2+} solution at pH = 5.0 to functionalized MOF resulted in the quenching of fluorescence at 580 nm due to the interaction between Hg^{2+} ion and sulfur-containing groups on MOF surface as well as electrostatic interaction. However, the addition of glutathione to this solution cause turn-on fluorescence due to the stronger interaction of this amino acid with mercury (II). Under optimal conditions, the calibration curve was linear in the concentration range

of 0.001-0.4 nmol L^{-1} for Hg^{2+} with a coefficient of determination of $R^2 = 0.9976$ and for glutathione in the range of 100-1000 µmol L^{-1} with a coefficient of determination of $R^2 = 0.9991$. The limit of detection (LOD = $3s_b/m$) and quantification (LOQ = $10s_b/m$) for Hg^{2+} was 0.0003 nmol $L^{-1}$and 0.0009 nmol L^{-1} and for glutathione were 2.90 µmol L^{-1} and 9.70 µmol L^{-1}, respectively. Inter-day and intra-day relative standard deviations (RSD%) **for determination of (n = 5)** for mercury (II) (0.1 nmol L^{-1}) were 2.2 and 4.1% and for glutathione (50.0 µmol L^{-1}) were 3.2 and 4.2%, respectively. **The method was successfully applied to the** determination of mercury (II) in water samples and glutathione in biological samples.

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Zinc Oxide−Graphene Nanocomposite-Based Transparent Surface Coating wth Antiviral Activity Against Herpes Simplex Virus

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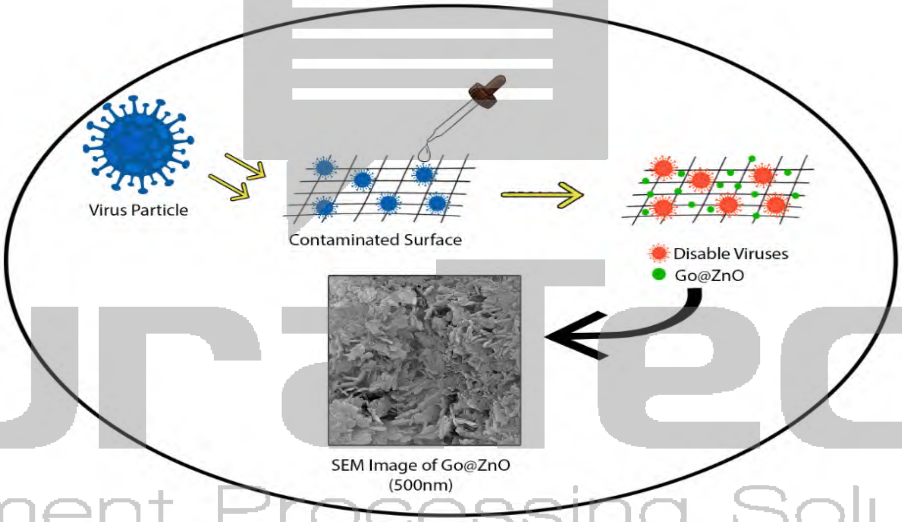
Graphical Abstract



Abstract: The emergence of novel virus strains and the associated outbreaks are becoming a significant threat to mankind.[1] Identifying the routes of transmission of the causative agent of diseases has an important role in controlling it. Viruses such as herpes simplex viruses, influenza viruses, and coronaviruses can be transmitted from infected to healthy individuals through contaminated surfaces, respiratory droplets, or contacts. An effective antiviral coating can decrease the viability of the virus particles in our surroundings significantly, hence reducing their transmission rate.[2] Extensive properties and biological characterization of nanocomposites,

graphene sheets, are available. It can inactivate virus particles in the shortest possible time and subsequently interfere with the entry of these virus particles into the host cell. This study aimed to produce a nanocomposite for virus inactivation on surfaces with stability of about one month. We have synthesized zinc Oxide- graphene oxide (ZnO−GO) nanocomposite as a material with the strong antiviral activity which retains its antiviral activity in liquid form and can therefore potentially be widely used to minimize contamination and microbial transmission on surfaces.

The synthesized nanocomposite was characterized by powder X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FT-IR). According to the scanning electron microscope analysis of ZnO-GO nanocomposite, the average particle size of the composite was 21.19 nm on the surface. By using HSV-1 as a model, the antiviral activity of ZnO−GO nanocomposites on the replication of the virus was investigated. The results of antiviral tests including Viral Plaque Assay and RT-qPCR; indicated that exposure with Zno−Go nanocomposites could suppress HSV-1 infection.

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Green Synthesis, Structural Characterization ZnO Nanoparticles Using salvia Officnalis Water Extract

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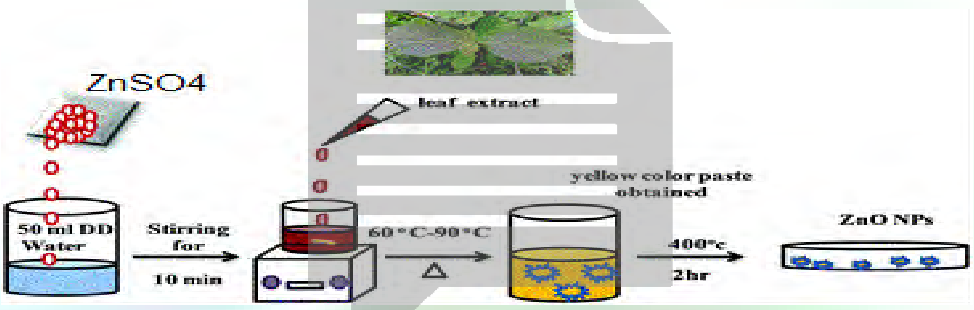
Graphical Abstract



Abstract: In recent years, biosynthesized zinc oxide nanoparticles (ZnO NPs) have been gaining importance due to their unique properties and tremendous applications. This study aimed to fabricate ZnO NPs by using extracts from salvia officnalisa traditional medicinal plant The various properties such as morphological, structural, and optical properties of green zinc oxide nanoparticles were characterized by Fourier Transform Infrared Spectroscopy, UV–Visible spectroscopy, Field Emission Scanning Electron Microscopy (FESEM), Energy Dispersive X-ray Spectroscopy and X-Ray diffraction (XRD). The XRD pattern revealed the crystalline nature of ZnO-NPs and the average diameter of particles is 20 nm. FESEM analysis show the spherical shape of ZnO-NPs with size ranging from 10 to 30 nm [1,2].

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Efficient Biosynthesis of Silver Nanoparticles Utilizing Jujuba Ziziphus Aqueous Leaf Extract

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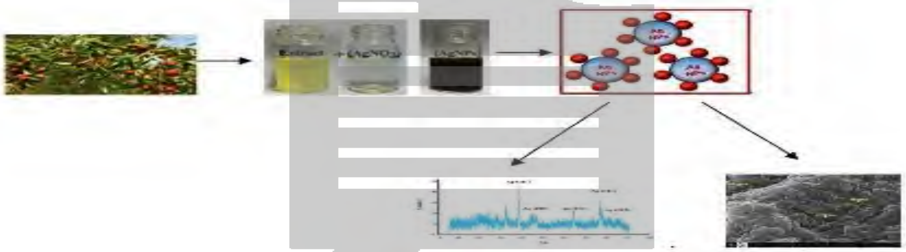
Graphical Abstract



Abstract: Silver nanoparticles (Ag NPs) were prepared via an inexpensive and eco-friendly manner from silver nitrate and deploying jujuba Ziziphus, plant extract as the precursor and reducing agent, respectively. Herein, an expeditious, green, facile, and eco-friendly synthesis approach is introduced and the synthesized nanoparticles' antibacterial activity was investigated; UV-Visible spectroscopy, XRD, SEM, and FT-IR were used to characterize silver nanoparticles. The characteristic absorption peaks were exhibited by ensued Ag NPs under UV-Visible spectroscopy as a result of SPR (surface plasmonic resonance) band in 415 nm wavelength, which was affirmed by FE-SEM images. The crystalline nature of Ag NPs was revealed by X-ray diffraction (XRD) results, whereas FE- SEM (25-40 nm) was used to calculate the size of nanoparticles. The functional groups responsible for the reduction of Ag+ ions to Ag NPs were displayed by the biosynthesized Ag NPs XRD pattern.

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Smartphone-Based Analysis in Environmental Analytical Chemistry: A Review

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Abstract: The possibility of environmental samples analyzing at the sampling's location is a special advantage that scientists have considered as the main goals in chemical and environmental analysis. The design of portable analytical devices facilitates this goal. Prevalent laboratory analysis tools are not portable, and the use of this equipment limits on-site analysis. Also, the use of these tools is sometimes unfavorable due to the production of hazardous waste, harmful radiation, and hazardous gases for the environment. Smartphones are the new aspect of modern life, and their application is becoming more and more widespread as advances in construction and enhancement of their capabilities. The significant increase in the use of these devices has been followed by the development and enhancement of various color detection modes to perform the needs of qualitative, semi-quantitative, and quantitative analysis. This article discusses the green aspects of various qualitative and quantitative analysis applications of smartphones, such as optical detection (colorimetry, fluorescence, chemiluminescence, bioluminescence, pixelation, and label-free detection), electrochemical detection, barcode reading, and imaging of smartphones with a fluorescence microscope. Also, its advantages and disadvantages in environment samples have been explained. Smartphone technique has been used for analysis of organic pollutants (Bisphenol A, Malondialdehyde,) and inorganic pollutants (Pb, Hg, Ni, Ca,…) in different environmental samples. This modern and popular technology could be a new turning point in environmental and analytical chemistry.

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Optimization of Efficient Removal of Lead Ions with Piperazine-Modified Magnetic Graphene Oxide (PIP@MGO) Nanocomposite Using RSM

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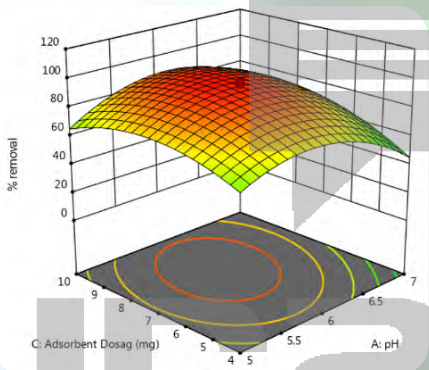
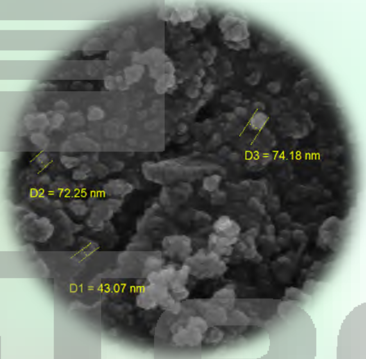
Graphical Abstract





Abstract: Disposal of industrial effluents and wastewaters is one of the most important challenges in the industrial world today. Among the various toxic metal ions, lead is a highly toxic pollutants that is released into the natural environment due to industrial activities. Acumination of Pb(II) ions inside the human body lead to various health consequences, therefore, in order to environmental clean-up, it is absolutely essential to design appropriate technologies for the completely elimination or reduce to an acceptable the level of Pb^{2+} ions. In the various treatment technologies, adsorption as a non-hazardous method is currently preferred for the heavy metal removal due to its many benefits. Graphene oxide (GO) as a single-layered two-dimensional nanomaterial has

aroused great interest between analytical chemists due to large surface area, high mobility and good conductivity. The dispersibility of GO nanosheets is very high and their separation from the solution medium is very difficult. To solve this problem and facilitate the separation after adsorption process, it is possible to create magnetic properties in graphene by making magnetic graphene nanocomposites.

In this research, the piperazine functionalized magnetic graphene oxide (PIP@MGO) nanocomposite was synthesized and used for the removal of Pb^{2+} ions. The physicochemical properties of adsorbent was characterized by XRD, FESEM, EDS, TGA, VSM and FT-IR analysis. In this method, the batch removal process were designed by response surface methodology (RSM) based on a central composite design (CCD) model. The results indicated that the highest efficiency was obtained from the quadratic model under optimum conditions of prominent parameters (pH = 6.0, adsorbent dosage = 70 mg, initial concentration of lead = 10 mg L^{-1}, and contact time = 30 min). Adsorption data showed that lead uptake followed the Freundlich isotherm model equation and pseudo-second order kinetic model. The maximum adsorption capacity was found to be 554.4 mg/g.

Keywords: Removal of Pb (II); Nanocomposite; Response surface method; Isotherms; Water treatment

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Smartphone-based Colorimetric Determination of Triclosan in Water Samples After Ultrasound Assisted-Dispersive Liquid-Liquid Microextraction Microextraction Under Optimized RSM Conditions

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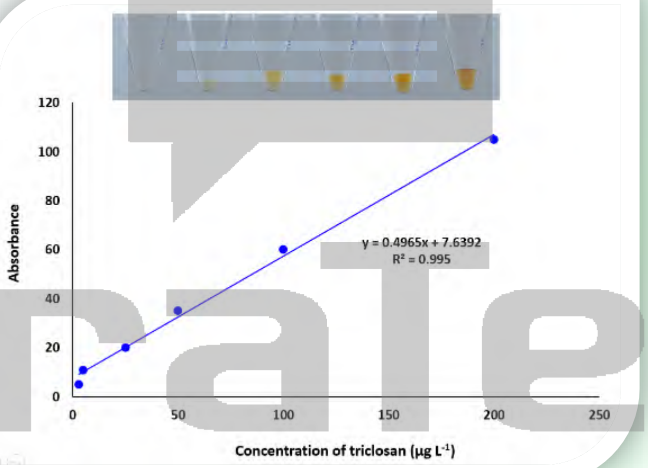
Graphical Abstract



Abstract: Triclosan (TCS), is widely used as antimicrobial and antifungal agent in personal-care products and consumer products. There are many reports of toxicity and risk of TSC to human health, and since 2016, the FDA and EEC prohibited the use of TCS in biocidal and antibacterial products. However, this contaminant is still used as an antimicrobial in other consumer products, and so TCS can be found in the environment. Hence, it is necessary to provide simple, sensitive and selective methods for extraction/pretreatment and then rapid detection of TCS in contaminated sources.

Currently, use of smartphones as cost-effective, easy-to-use and portable devices for advanced colorimetric detection is emerging as a powerful analytical tool. This capability has greatly increased in recent years due to the increase in camera quality and the improvement of their electronic equipment's.

In the present study, a simple and low cost methodology based on ultrasonic assisted- DLLME followed by smartphone-based colorimetric measurement was introduced for the separation and determination of TCS. This method is based on the formation of an azo compound from the alkaline reaction of TCS with a diazonium ion resulting from the reaction of sodium nitrite and p-sulfanilic acid in an acidic medium. The produced orange-yellow color is extracted in a low volume of organic phase by UA-DLLME and RGB values are recorded with *Color Grab* app to measure its absorbance. The effective parameters namely solution pH, concentration of *p*-sulfanilic acid and nitrite, reaction time and extraction solvent volume were investigated and optimized by response surface methodology (RSM) based on a BBD model. The calibration curve was linear in the range of 5.0 and 300 μg L^{-1} of TCS and limit of detection (LOD) was 1.2 μg L^{-1}. Then, the proposed method was successfully used for the analyses of triclosan in several environmental water and wastewater samples and satisfactory results were obtained.

Keywords: Triclosan; Smartphone; RGB data; Ultrasound Dispersive liquid-liquid microextraction; Color Grab

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Separation of Cationic Dyes Using a Green Emulsion Liquid Membrane Based on Non-Ionic Polysorbate Surfactants

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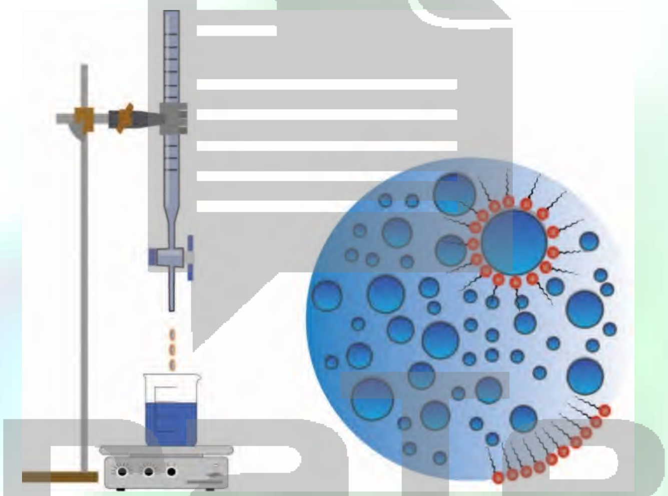
Graphical Abstract



Abstract: In the present research, the stability and extraction rate for cationic dyes using two non-ionic surfactants, polysorbate 20 and 80, in an emulsion liquid membrane containing edible green solvent were investigated. The ELM phase was prepared using several concentrations of the surfactants, D2EHPA as the carrier, and NaOH as the internal phase. The effects of surfactant concentration, carrier concentration, and stirring speed at extraction stage and the stability of the membrane phase were studied. The results showed that at an optimum condition, a separation of more than 90% could be achieved for cationic dyes using green ELM.

Treatment of Oil Effluents by Microbial Electrolysis Cell (MEC) Method in Comparison with Activated Sludge Process (ASP)

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Graphical Abstract

Abstract: Due to the increasing demand and globalization of the use of oil resources and other energy sources, the production of petrochemical wastewater has been increased, so that in 2016 the production rate of oil wastewater was reported 5.06×10^7 t/d. Discharge of these wastewater without elimination of hydrocarbons is dangerous for the environment. Therefore, efficient treatment of petrochemical wastewater is necessary to overcome the challenges that arise. In addition, water management is necessary .Currently, physicochemical (Physical-chemical) methods are commonly used to treat petrochemical wastewater that have limitations such as high investment, high operating costs, production of hazardous sludge, and saline solutions, as well as the need for skilled labor. These disadvantages lead to increased attention to the use of biological methods .The biological methods used are Activated Sludge process (ASP) and Microbial Electrochemical Techniques (MET). METs can simultaneously treat wastewater and produce useful products. One of the types of METs is Microbial Electrolysis Cells (MEC). Unlike ASP,

Microbial Electrochemical Techniques don’t require much ground and aeration and are cheaper, they also don’t produce odors. In this study, the performance of Activated Sludge Method with Microbial Electrolysis Cell against oil wastewater was investigated. To do this, 30% (volumetric / volumetric) of wastewater was added to the BHI medium, one in ASP mode and the other in Single-Chamber Microbial Electrolysis Cell (SMEC) with voltage of 0.8 v, and the chambers were filled with a mixture of N_2/CO_2 gases. After 48 hours, the environment at MEC was clearer and contained more sediment. The use of METs is more efficient than the ASP method because the elimination process is done more and the technique has the potential to produce valuable products such as electricity and hydrogen and methane gases.

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Environmental Risk Assessment of Heavy Metals in Road Dust of Isfahan Metropolitan

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Graphical Abstract

Abstract: Heavy metals (HMs) are one of the main pollutants in the environment, which have adverse environmental and health effects. Therefore, their risk assessment is an important

environmental issue. In this study, the environmental risk of 6 HMs including Pb, Co, As, Ni, Cr and Cd in road dusts of 4 sampling stations (Jomhori Square, Azadi Square, Segzi and Gavkhuoni Wetland) was investigated. The ecological risk of metals was assessed using the pollution index (PI), enrichment factor (EF) and geo-accumulation index (I_{geo}) as well as pollution load index (PLI). The health risk of each metal was assessed separately in two cases of carcinogenic risk and non-carcinogenic risk for adults and children. The mobility of each metal was calculated using the Mobility Factor (MF) index. The results of PI, EF and I_{geo} indices showed that Cr and Ni had the highest and lowest risk, respectively. Besides, the results of PLI showed that Jomhori Square and Azadi Square stations were more polluted than the other stations. According to the results of health risk assessment, Cr and Cd showed the highest non-carcinogenic risk, whereas among the elements, the carcinogenic risk of Cr exceeded the carcinogenic risk limit. The mobility of elements followed the decreasing trend of Pb> Ni> Co> As> Cd> Cr. Considering the results, management and prevention of road dusts and particles are highly recommended.

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Ultrasound-Assisted Dispersive Liquid-Liquid Microextraction Combined with iIon Mobility Spectrometery for The Determination of Chlorpyrifos

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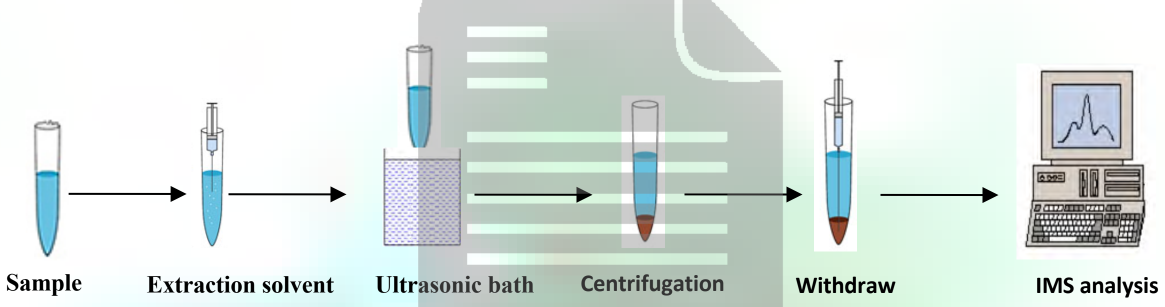
Graphical Abstract



Abstract: Chlorpyrifos is an organophosphorus pesticides (OPPs) extensively applied to improve the quality and quantity of agriculture product owing to their high efficiency relatively and low persistence in the environment. However, the consumedly use of OPPs could generate serious contamination to the environment, and endanger human health due to the inhibition of the acetylcholinesterase activity in the nervous system. Therefore, it is very important to develop a fast, simple, sensitive and reliable analytical method for monitoring of OPPs residues in various samples including food, environmental and biological matrixes. In this work an ultrasound-assisted dispersive liquid-liquid microextraction method (US-DLLME) was developed for the extraction and preconcentration of chlorpyrifos prior to its determination by ion mobility spectrometry (IMS). The laboratory factor affecting the extraction efficiency such as pH, type and volume of extraction solvent, ultrasound time, centrifuge time, ionic strength and volume of aqueous phase were examined and optimized. Under the optimum conditions, the calibration curve was linear in the range of 15 – 350 μg L^{-1} ($R^2 = 0.9995$). Limit of detection (LOD) based on $3S_b/m$ (where m is the slope of calibration graph and S_b is the standard deviation of blank solution) was

obtained 5 μg L^{-1}. The developed US-DLLME procedure was successfully employed for the determination of chlorpyrifos in tap water and well water samples. The accuracy of the proposed method was examined through the relative recovery determination by spiking the real samples with two levels of chlorpyrifos. The results of this analysis showed that the calculated recoveries were obtained from 94 to 101.7%.

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Dispersive Liquid-Liquid Microextraction Technique Based on Solidification of Floating Organic Drop for Preconcentration and Determination of Molybdenum in Water Samples Prior to Uv-Visible Spectrophotometry

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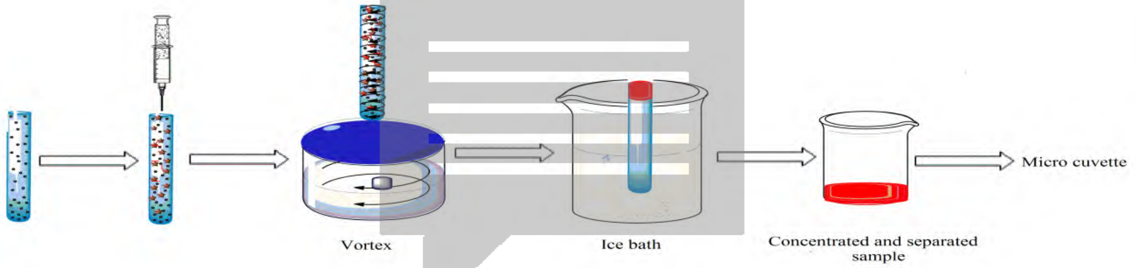
Graphical Abstract



Abstract: Molybdenum is a biologically and environmentally relevant trace element. It possesses variable oxidation states, ranging from +2 to +6, easily convertible into each other. However, the concentration levels in these kinds of samples are usually low, in the µg kg range. Thus, highly sensitive techniques are required, namely, electrothermal atomic absorption spectrometry associated with a preconcentration step, in order to achieve better detection limits [1]. In this work, a novel method based on dispersive liquid-liquid microextraction technique based on solidification of a floating organic drop prior to UV-Vis spectrophotometry for determination of molybdenum at trace levels in environmental samples is proposed. The method is based on the reaction of Mo with thiocyanate (SCN^-) as a chelating agent for formation of $Mo(SCN)_5$ in acidic medium. An appropriate mixture of acetone and 1-undecanol was rapidly injected into an aqueous sample and the color red complex of molybdenum is then extracted with 1-undecanol. After centrifugation, the test tube was cooled for 5 min and the solidified 1-undecanol drop formed on the top of the solution was transferred into a micro-cuvette to be determined by UV-Vis spectrophotometry. Absorbance of the complex was measured at 470 nm. Several important relevant parameters such as the amount of 1-undecanol and acetone, concentration of sulfuric acid and extraction time have been investigated. Under optimum operating conditions, the calibration curve was plotted which was linear in the concentration range of 12 to 100 ng mL^{-1} of Mo. The limit of detection (LOD) of the method was obtained to be 3.8 ng mL^{-1} based on 3sb/m. The relative standard deviation (RSD%) of the method was found to be 3.3% for ten replicate measurement.The proposed method

has been successfully applied for the determination of the Molybdenum in tap and well water samples with recoveries in the range of 95-103%.

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A New Fluorescent Chemosensor Based on 1-Benzylidene Thiosemicarbazide for Sensitive Detection of Silver Ions

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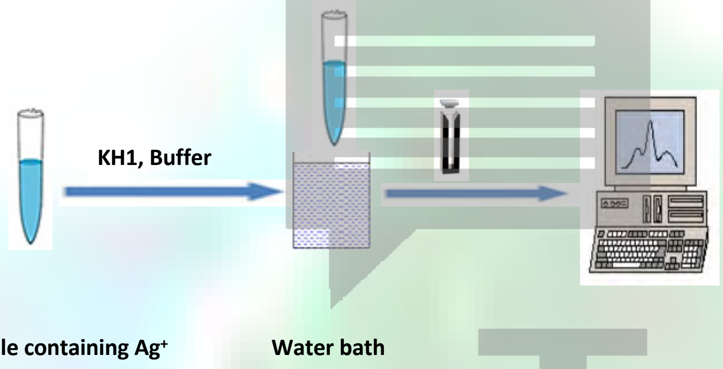
Graphical Abstract



Abstract: Silver (Ag) is a precious metal widely used in various industrial fields including electronics, catalysis, photography and imaging due to its unique chemical and physical properties. Also, silver has an important role in medical science including application as antibacterial cream or antibiotic coating on medical devices such as catheters owing to its antibacterial properties. However, silver can coordinate with some metabolites including imidazole, carboxyl, amino and thiol functional groups in proteins/enzymes. Hence, it can be deactivate protein/enzyme function in the human body which can cause many symptoms and diseases. Therefore, development of a simple, sensitive, fast and selective analytical method for monitoring of silver concentration in environment and human body is great of attention. Currently, determination of silver is based on conventional techniques such as inductively coupled plasma optical emission spectrometry, atomic absorption/emission spectroscopy,

inductively coupled plasma-mass spectrometry, surface-enhanced Raman spectroscopy, electrochemical and microextraction methods and fluorescence spectroscopy.

In this work, a new Schiff base named as 1-benzylidene thiosemicarbazide (KH1) was successfully synthesized and was used as a sensitive and selective chemosensor for determination of trace amount of silver ion (Ag^+). The fluorescence intensity enhanced by increasing silver ion concentration at 351 nm. Experimental parameters affecting the fluorescence intensity such as pH, type of solvent, concentration of KH1, temperature and reaction time were studied and optimized. In addition, the synthesized probe exhibited good selectivity for Ag^+ compared to other metal ions such as Co^{2+}, Na^+, K^+, Cd^{2+}, Ba^{2+}, Cr^{3+}, Zn^{2+}, Cu^{2+}, Ni^{2+}, Ca^{2+}, Al^{3+}, Fe^{2+}, Hg^+, Mn^{2+} and Mg^{2+} in aqueous solution.

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Removal of Methylene Blue by Using of Vanadium-Carbon Nanocomposite

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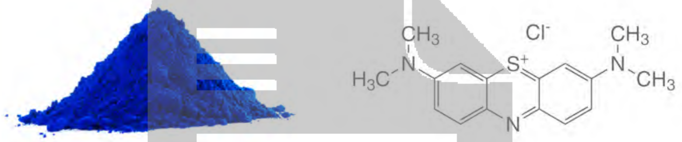
Graphical Abstract



Abstract: Methylene blue is the most common dye used to dye cotton, wool and silk. Inhalation of this compound can cause respiratory distress, while direct exposure to it can cause permanent damage to the eyes of humans and animals, local burns, nausea and vomiting, increased sweating, mental disorders and methemoglobinemia. Effluents containing dyes such as methylene blue are hazardous to ecosystems and public health; these substances may affect the light activity of aquatic plants, increase suspended solids, and water turbidity by reducing light penetration. In addition, dyes are carcinogenic and mutagenic to humans. Therefore, considering a suitable treatment method according to existing standards is necessary and inevitable.

In the current work, for the first time, vanadium oxide / carbon nanocomposite has been used as an adsorbent for removal of methylene blue. The performance of this nanocomposite in removal of methylene blue dye from aqueous media was studied. In this manner, effect of various parameters such as pH, adsorbent amount, contact time and solution concentration on the removal of methylene blue were examined. The results show that the maximum amount of was observed at pH 3.0 and 60 min. Also, the maximum amount of adsorption capacity is 0.4 mg / g. On the other hanf, different adsorption isotherms were implemented for analysis of experimental data. In this way, Langmuir model presented best fitted lines which shows the monolayer adsorption process and the presence of specific homogeneous site within the adsorbent.

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Rapid and Naked-Eye for Colorimetric Detection of Morphine Sulfate, Using Silver Nanoprobe

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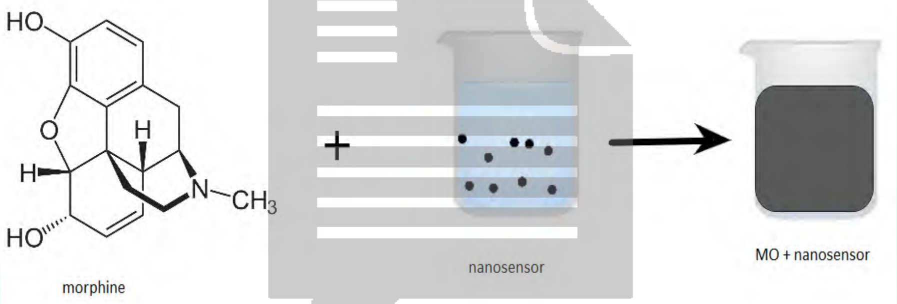
Graphical Abstract



Abstract: morphine (MO) is one of the most widely used drugs in the world, and its timely and accurate identification is of particular importance [1]. This study presents a new and simple colorimetric method for sensitive and visual detection of MO in urine using silver nanoparticles [2]. The structure and properties of nanosensors were investigated using XRD, UV-VIS, TEM analyzes [3] [4]. To the best of our knowledge, this is the higher the concentration of the drug caused more discoloration [5].

The bonding interactions between the nanosensor and MO cause AgNPs to accumulate [6], resulting in a color change from yellow to smoky, which can be detected by the naked eye [7]. To evaluate the LOD level and quantitative measurement of MO, different concentrations of MO were prepared and analyzed with a synthesized nanosensor [8] [9].

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Highly Sensitive Colorimetric Nanosensor for Quantitative and Qualitative Detection of Methamphetamine

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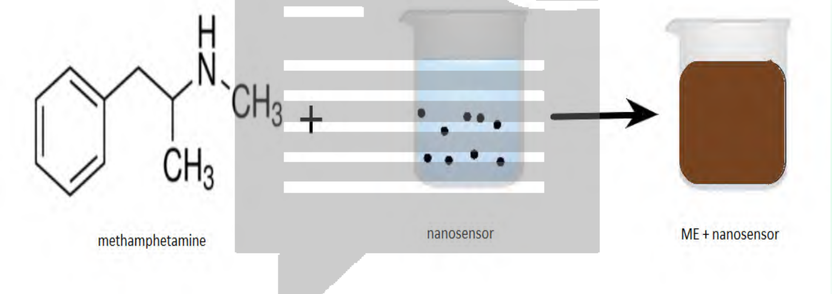
Graphical Abstract



Abstract: Methamphetamine (MA) is one of the most widely used drugs in the world, and its timely and accurate identification is of the particular importance [1]. This study presents a new and simple colorimetric method for sensitive and visual detection of MA in urine using silver nanoparticles. [2] The structure and properties of nanosensors were investigated using XRD, UV-VIS, TEM analyzes. [3] To the best of our knowledge, this is the higher the concentration of the drug caused to the more discoloration [4].

The bonding interactions between the nanosensor and MA cause AgNPs to accumulate, resulting in a color change from yellow to brown, which can be detected by the naked eye[6]. To evaluate the LOD level and quantitative measurement of MA, [7] different concentrations of MA were prepared and analyzed with a synthesized nanosensor [8] [9].

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Orange Peel Derived Carbon Nanospheres Decorated by Manganese Oxide Nanosheets, Intercalated Into Polypyrrole, As an Inside-Needle Capillary Adsorption Trap Sorbent For Analysis Of Linear Alkylbenzenes

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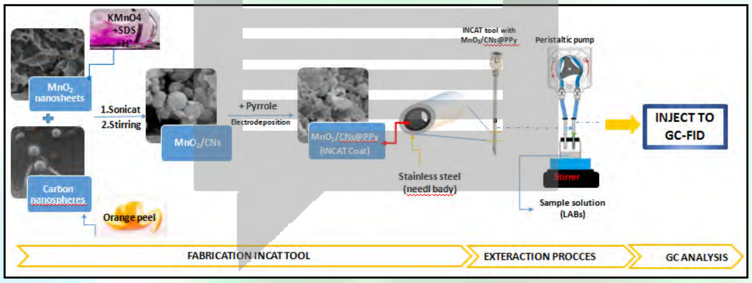
Graphical Abstract



Abstract: Carbon nanospheres (CNSs) were derived hydrothermally from biomass (orange peels) and decorated by manganese dioxide (MnO_2) nanosheets. The MnO_2/CNSs nanocomposite was intercalated into polypyrrole (PPy) during flow-through in-situ electropolymerization of pyrrole on the surface of the inner wall of a stainless-steel needle to preparing inside-needle capillary adsorption trap (INCAT) device. The surface morphology, sorption characteristics, and structure of the MnO_2/CNSs@PPy nanocomposite were characterized using scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), nitrogen absorption by the Brunauer-Emmett-Teller (BET) method, dynamic light scattering (DLS) size distribution, and Fourier-transform infrared spectrometry (FT-IR). The INCAT tool was coupled with GC-FID and applied for dynamic headspace perconcentration and determination of linear alkyl benzenes (LABs) in wastewater samples. Optimization of the main effective experimental variables of the proposed

method was carried out using a central composite design (CCD) based on response surface methodology (RSM). Under the optimal conditions, the limits of detection (LODs) and limits of quantification (LOQs) were 0.5-1.0 and 10-15 ng mL^{-1}, respectively, and the calibration plots were linear over the range of 0.015–10 µg mL-1.The relative standard deviations (RSDs%) for intra-day, inter-day, and inter-INCAT precision were calculated to be 6.5, 11.7, and 15.2%, respectively. The developed technique was employed successfully for the extraction and determination of LABs in water and wastewater samples with average recovery values ranging from 92-109%. The superiority of the adsorbent for separation and preconcentration of LABs was demonstrated by its comparison with other INCAT tools. A single INCAT device was used more than 90 times without significant change in its extraction capability.

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Post-Illumination Catalytic Memory Nanophotocatalyst Of Ag Doped SrTiO3 For Degradation Dye

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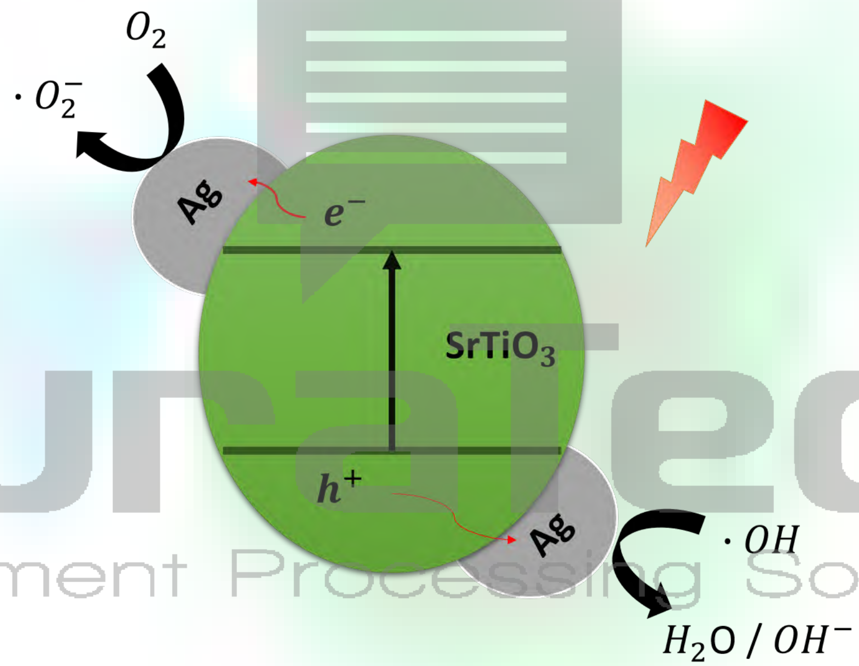
Graphical Abstract



Abstract: $SrTiO_3$ as a perovskite structure has low cost, excellent stability, long service life, large surface area, low toxicity, and high photocatalyst activity.[1] Recently the studies are achieved the distinctive photocatalyst with memory effect, which can retain catalyst performance in the dark. Photocatalysts with memory effect recently have attracted a lot of attention for their ability to retain excellent catalytic efficiency in the dark.[2] Electron storage capacity limited, as a result the activities of photocatalyst with memory effect are low.[3] Thus, $SrTiO_3$ doping with cations such as Ag can alter electronic properties which have the capacity to storage electrons increases photocatalytic activity. In this study, we prepared sonochemical method for synthesis of Ag doped

$SrTiO_3$ to investigate the photocatalytic with memory effect to degradation the dye. We fabricated Ag doped $SrTiO_3$ nanophotocatalyst by doping $SrTiO_3$ with Ag. Ag doped $SrTiO_3$ nanophotocatalyst performed very well in degradation the dye pollutant under light and post-Illumination. The effect of temperature, pH, amount of nanophotocatalytic material and concentration of dye solution on the efficiency of photocatalytic activity was examined. Ag doped $SrTiO_3$ nanophotocatalyst were characterized by X-ray diffraction (XRD), ultraviolet-visible diffuse reflection spectroscopy (UV–vis), transmission electron microscopy (TEM), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR).

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Green Synthesis of Iron Oxide Nanoparticle Using *Pistacia vera L.* Leaves Extract and Its Antibacterial Activity

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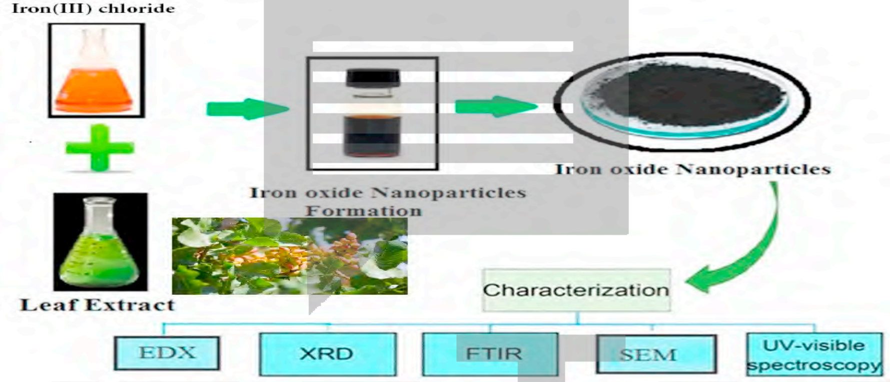
Graphical Abstract



Abstract: Synthesis of iron oxide nanoparticles by the recently developed green approach is extremely promising because of its non-toxicity and environmentally friendly behaviour. In this study, nano scaled iron oxide particles (α-Fe_2O_3) were synthesized from hexahydrate ferric chloride ($FeCl_3.6H_2O$) with the addition of *Pistacia vera L.* leaves extract under atmospheric conditions. The synthesis of iron oxide nanoparticles was confirmed by systematic characterization using UV, FTIR, XRD, FESEM and EDX studies The synthesized nanoparticles showed moderate antibacterial activity against E.Coli bacterial strain.

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Visible-light Nanocomposite Photocatalyst Of $SrTiO_3/g\text{-}C_3N_4$ For Degradation Dye

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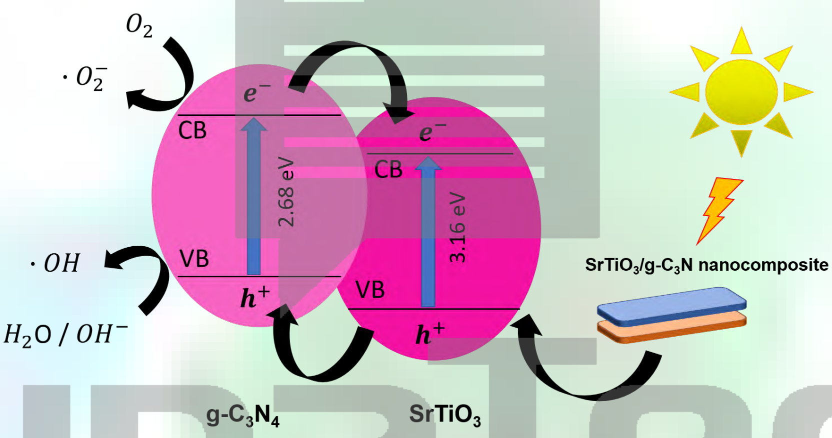
Graphical Abstract



Abstract: Semiconductor photocatalysts for environmental applications can be composite with other semiconductors to be activated in a wide range of light.[1] The recent reports show that nanocomposite photocatalyst material semiconductors with narrower bandgap, improve photodegradation efficiency in visible light irradiation.[1] This makes photocatalytic nanocomposites applicable in many fields such as the environment. Recently photocatalyst with memory effect has appreciable attention because of the unique talent to keep the catalytic efficiency in dark conditions.[2,3,4] Post-illumination catalytic memory achieves the degradation of dye in the dark.[3,4] The nanocomposite photocatalyst could store a portion of its photoactivity via photogenerated electrons under visible light irradiation and then release the electrons again in the dark. Graphitic carbon nitride ($g\text{-}C_3N_4$) as efficient photocatalyst and strontium titanate ($SrTiO_3$) as super capacitor (perovskite structure) have relatively unique physiochemical properties, large surface area, low price, and long service life, ease of synthesis, product scalability, controllable bandgap properties, low toxicity, and high photocatalytic activity and unique optical-electronic properties. [3,4,5] In this study, we investigated the sonochemical method for the synthesis of visible light-activated nanocomposite photocatalyst with $SrTiO_3$ and $g\text{-}C_3N_4$. As-prepared $SrTiO_3/g\text{-}C_3N_4$

reduced bandgap meanwhile activated under visible light and used as a supercapacitor electrode material. The hybrid nanocomposite $SrTiO_3/g\text{-}C_3N_4$ shows an improved photocatalytic activity and photocatalyst response under visible light irradiation and dark condition. Also, we examined effects of pH, temperature, amount of nanocomposite photocatalytic material and concentration of dye solution. The results obtained in this study show that nanocomposite photocatalyst $SrTiO_3/g\text{-}C_3N_4$ can degrade the dye pollutant. The as-prepared $SrTiO_3/g\text{-}C_3N_4$ nanocomposites were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), ultraviolet-visible diffuse reflection spectroscopy (UV–vis).

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Green Synthesis and Characterization of Zinc Oxide Nanoparticles using *Pistacia vera L* Skin Aqueous Extract and Its Antibacterial Activities

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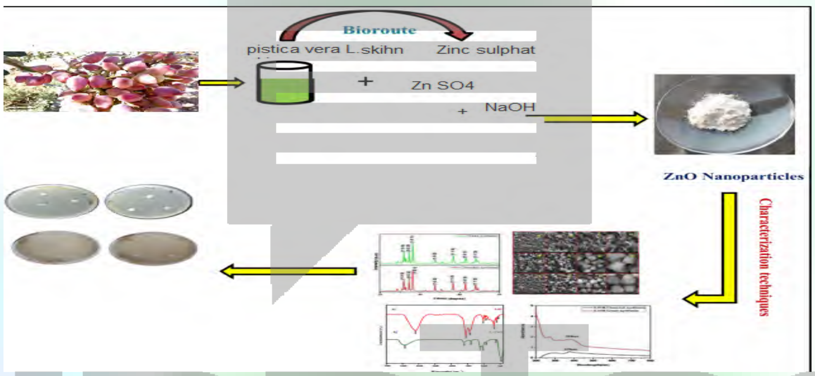
Graphical Abstract



Abstract: Development of plant based nanoparticles has many advantages over conventional physico-chemical methods and has various applications in medicine and biology. In present study, zinc oxide (ZnO) nanoparticles (NPs) were synthesized using Pistacia vera L skin ectract. 0.01 M zinc sulphate was used as a precursor in extract for NPs synthesis. The structural and optical properties of NPs were investigated by X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, scanning electron microscope(FESEM) and ultraviolet-visible spectrophotometer (UV-Vis) . The antibacterial potential of ZnO NPs was examined by paper disc diffusion method against two clinical strains of Escherichia coli (E. coli) based on the zone of inhibition and minimal inhibitory indices (MIC). Change in color of the reaction mixture from brown to white indicated the formation of ZnO NPs. UV peaks at 320 nm , and XRD pattern matching that of JCPDS card for ZnO confirmed the presence of pure ZnO NPs. FTIR further confirmed the presence of bioactive functional groups involved in the reduction of bulk zinc sulphate to ZnO NPs. SEM analysis displayed the shape of NPs to be spherical whereas showed their size range from 30 to 78 nm.

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One-pot and Green Synthesis of Tetrahydrobenzo [b] Pyran in The Presence of Catalyst Heteropolyacid Supported on Graphite Carbon Nitride

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Graphical Abstract

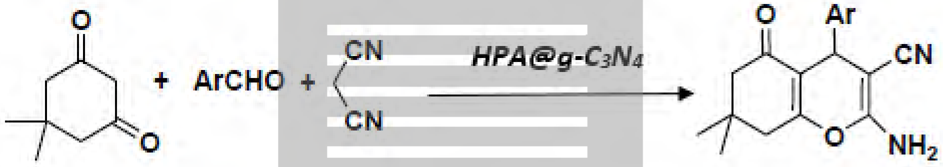

Figure 1. Synthesis of tetrahydrobenzo [b] pyran compounds using HPA @ g-C3N4 nanocatalyst

Abstract: Benzopyrans are of interest due to their wide range of biological and medicinal properties. In this paper, a suitable high-performance, functional method for the synthesis of tetrahydro benzo [b] pyran with the use of aromatic aldehydes, malononitrile, and dimedone is developed. The heteropolyacid supported on graphite carbon nitride was studied as a catalyst and water as a green and environmentally friendly solvent. In this method, in addition to excellent performance in environmental conditions, it has advantages such as short reaction time, mild reaction conditions, use of non-toxic catalyst, high efficiency of products. Also, the catalyst can be easily and effectively recovered without Loss of catalyst activity can be reused.

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Ion Pair Solvent Bar Microextraction Prior to UV-Vis Spectrophotometry for Determination of Paraquat

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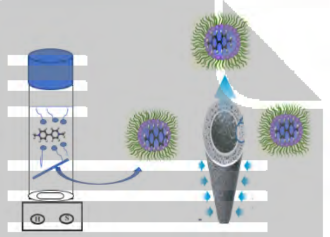
Graphical Abstract



Ion pair solvent bar micro extraction schematic

Abstract: A group of quaternary ammonium compounds, also known as quats, have been used as herbicides and anticholinergic drugs [1]. Among quats, paraquat (PQ) is a very quick acting herbicide for broadleaf weed control in fields[2]. Because the use of PQ results in pollution of surface and river water, it is essential to develop a rapid and accurate method for determining these compounds in environmental samples [3]. Due to the permanent ionic character of quats, these herbicides are highly hydrophilic. Ion pair extraction is a suitable method for the partitioning of ionic and hydrophilic species with the help of counter ions of opposite charge in SBME systems [4]. The ion pairing agent can be added to the donor solution before the extraction process or be dissolved in the membrane organic phase to form a neutral ion pair complex [5]. From this perspective, surfactants can be used as effective ion pairing reagents to achieve this purpose. In this work, for the first time, a new analytical method based on ion pair solvent bar microextraction (IP-SBME) was introduced. In this two phase process, an anionic surfactant (SDS) was added initially into the donor solution to form a hydrophobic ion pair with the cationic analyte. Thereupon, the ion pair formed was enriched into organic solvent immobilized in the pores and lumen of the HF (toluene) and finally back washed with methanol. At optimum conditions, value of variables were set as pH 6, concentration of SDS 4 mM, stirring rate of 400 rpm, time of extraction 15 min, without addition of salt. Under the optimized extraction conditions, the method showed a good linear dynamic range (1–2000 ugL^{-1}) with a lower limit of detection (0.3 ugL^{-1}) and excellent preconcentration factor (PF =355.34). Finally, the proposed method was successfully applied for the determination of PQ in soil samples.

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Study of Acid Red 1 Removal from Aqueous Solution by Photo-Fenton ($UV/Fe^{2+}/H_2O_2$) Process

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Abstract*:* Removing colored contaminants from the wastewater output of various industries (such as textile and paint) is the main concern of environmental protection. Regardless that the presence of such pollutants creates an unpleasant appearance, it also may cause irreversible threats to flora and fauna. For example, accumulation of colored pollution in water resources may disrupt the nutrition of aquatic biota. Acid red 1 (AR1), which was chosen as the model compound in the present investigation, is a synthetic red azo dye. Azo dyes are the largest class of aromatic dyes having lots of commercial interest. These dyes are mostly used in textile industries. Several physico-chemical techniques have been developed to remove colored contaminants which, of course, the use of simple and efficient methods is crucial. The literature review showed that advanced oxidation processes (AOPs) are useful methods for the removal of various contaminants, especially colored compounds. The aim of this research was to study the remove of AR1 dye from aqueous solution by Photo-Fenton ($UV/Fe^{2+}/H_2O_2$). Effect of four operational variables viz. initial dye concentration, Fe_2O_3 amount, pH, and time was studied in Photo-Fenton process. Modeling and optimization of process was studied using response surface methodology (RSM). Comparing of the theoretical and experimental results showed that the results are in good agreement with each other, which is supported by analysis of variance (ANOVA). Two and three-dimensional graphs (contours and response surfaces) were used to assess the interaction between operational parameters. The findings demonstrated that, removal efficiency decreased with increasing of initial

dye concentration, while it increased with increasing of Fe_2O_3 and H_2O_2 amounts. It also turned out that, removal efficiency increased with increasing of pH and irradiation time.

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Preparation, Optimization and Characterization of Chitosan from Different Shells of Bushehr Sea Shrimp and Its Comparison with Commercial Samples

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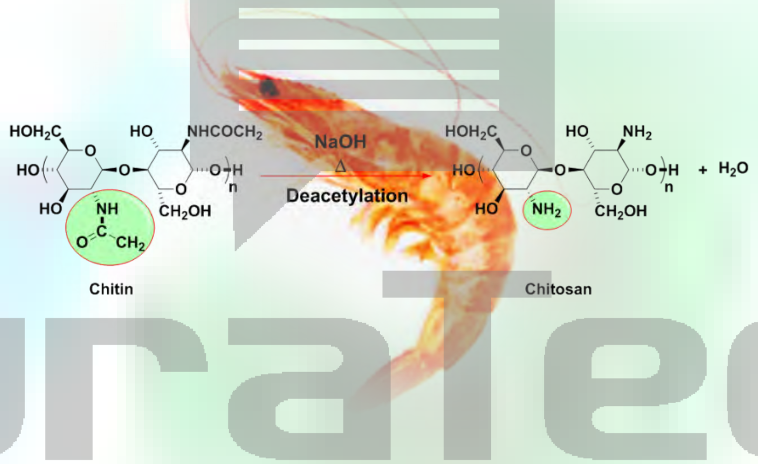
Graphical Abstract



Abstract: Every year, about half or more (40-70%) of marine crustaceans, especially south sea aquatic animals, are disposed of as waste. It should be noted that aquatic waste, especially shrimp skin, as valuable wastes can be used to synthesize substances such as chitin and chitosan. Among the mentioned lesions, 20 to 30% of the external skeleton of these aquatic animals, especially crustaceans, is chitin. It is worth mentioning that, this substance is present in the structure of many edible fungi as well as plants such as yeasts and insect cuticles. By removing the acetyl groups in the chitin molecule, its most important derivative, chitosan, can be synthesized. This process was first developed by Rouget in 1859 through the base deacetylation of the chitin in the presence of potassium hydroxide, leading to the conversion of acetyl amine groups in chitin to amine agents and the eventual discovery of chitosan. Today, according to the contract, the number of acetyl groups in the chain determines the difference between these two polymers, and according to this contract, the presence of 50% of amide groups is considered as the boundary between chitin and chitosan, ie polymers with less than 50% are called chitin and more than 50% is called chitosan.

Important parameters such as degree of acetylation, molecular weight and crystallinity can affect the physical and chemical properties of chitin and chitosan. [1-4]

Currently, the most important source for economically viable extraction of chitosan is the crustaceans of marine such as shrimp, crabs and krill. Chitosan can be used in the release of drugs, hemodialysis, artificial skin, meat and dairy additives, the chelating agent of heavy metal ions in wastewater treatment, and the separation of nucleic acid in thin layer chromatography. Also, due to a large number of functional groups in chitosan, it is possible to mix this polymer with a wide range of polymers. [5-7]

The purpose of this report is to prepare, optimize and characterize chitosan from different shells of Bushehr marine shrimp and compare it with commercial samples through HNMR, XRD, FE-SEM, and FT-IR spectroscopy.

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Polyacrylamide Modified Salep as A Natural Superabsorbent

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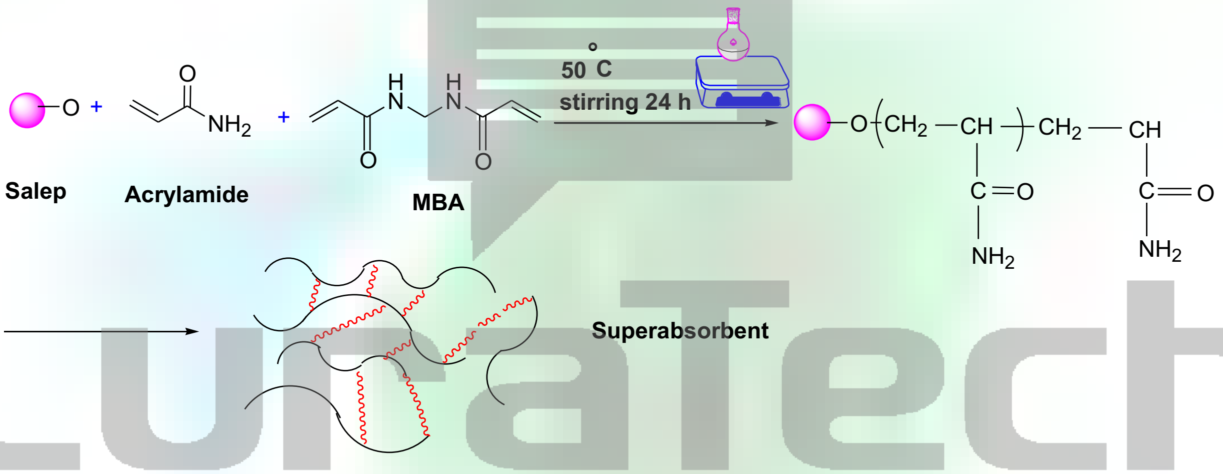
Graphical Abstract



Abstract: Superabsorbent polymers (SAP) are a class of polymeric materials that have the ability to absorb and retain a large amount of water in aqueous solutions [1]. SAPs are a unique class of three-dimensional cross-linked polymeric networks and are used in various fields [2]. In this study, modified salep with polyacrylamide was used as a superabsorbent. Free radical polymerization and reversible addition fragmentation polymerization methods were applied to modified salep [3]. Polyacrylamide was cross-linked by a curing agent and the obtained hydrogel had better strength and the water absorption capacity increased. Swelling measurements show that the water absorption rate has increased to 3020 %. the characterization will also be done by FT-IR, SEM, TEM, TGA, … analysis.

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Use of Cost-Effective Untreated Biomasses as Potential Biosorbents for Formaldehyde Removal from Wastewater

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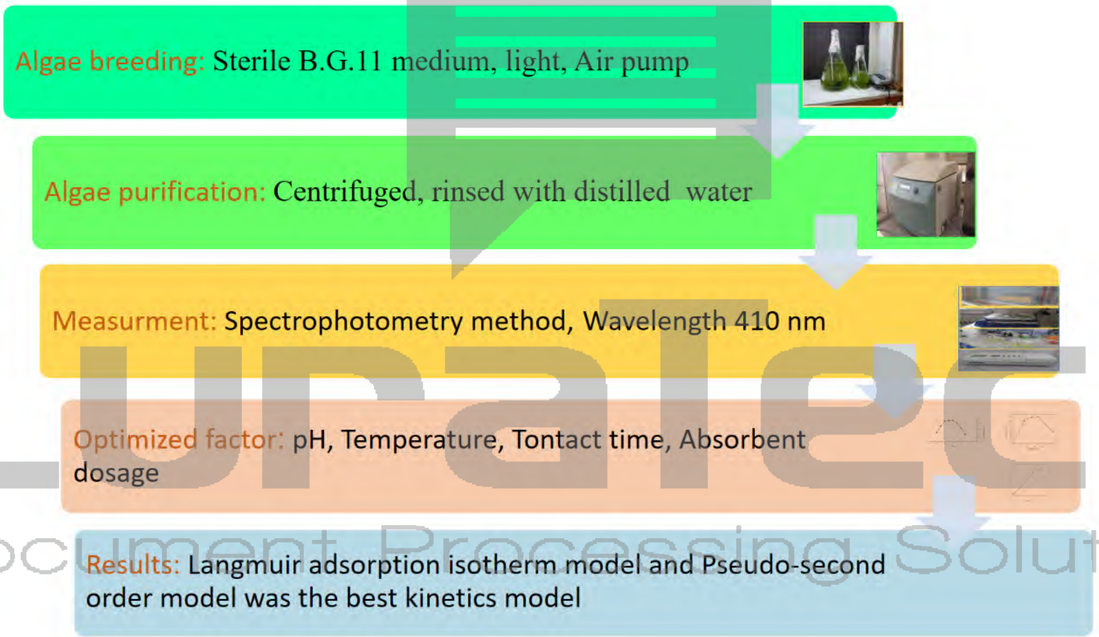
Graphical Abstract



Algae breeding: Sterile B.G.11 medium, light, Air pump

Algae purification: Centrifuged, rinsed with distilled water

Measurment: Spectrophotometry method, Wavelength 410 nm

Optimized factor: pH, Temperature, Tontact time, Absorbent dosage

Results: Langmuir adsorption isotherm model and Pseudo-second order model was the best kinetics model

Abstract: Formaldehyde is a toxic and dangerous compound that is considered as one of the carcinogenic and mutagenic agents in organisms [1]. Formaldehyde is used in many industrial activities such as the production of adhesives and resins, paper, and pharmaceuticals [2-4]. The toxicity of formaldehyde to microorganisms limited its removal by aerobic biological methods. In this study, the ability of the alga Chlorella Vulgaris in removal of formaldehyde was investigated. In this regard, Chlorella Vulgaris was grown in a sterile B.G.11 medium. It was then centrifuged; the algae were separated from the culture medium and rinsed several times with distilled water. The amount of formaldehyde was measured by the spectrophotometry method. Parameters affecting the removal of formaldehyde such as contact time, temperature, and pH have been

investigated and optimized. The sorption isotherms and analytic kinetics with biosorbent were investigated using linear and nonlinear regression. Under the optimized pH of 6.0, Chlorella Vulgaris Microalgae was able to remove 98 % of formaldehyde within 10 minutes. The equilibrium sorption experiments were evaluated by Langmuir, Freundlich, Tempkin, and Dubinin-Raduskovich isotherm models. The sorption kinetic were studied by pseudo-first-order, pseudo second order, Elovich, and intra-particle diffusion. The sorption isotherm followed Langmuir isotherm and the kinetics of the sorption followed the pseudo-second-order model. The maximum monolayer sorption capacity of Chlorella Vulgaris based on Langmuir model was found to be 158 mg g^{-1}. Rapid and relatively high capacity of natural and untreated Chlorella Vulgaris Microalgae is the main advantage of this biosorbent for wastewater treatment.

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Standardization of Dispersive Liquid-Liquid Microextraction for Determination of 16 Polycyclic Aromatic Hydrocarbons in Water Samples

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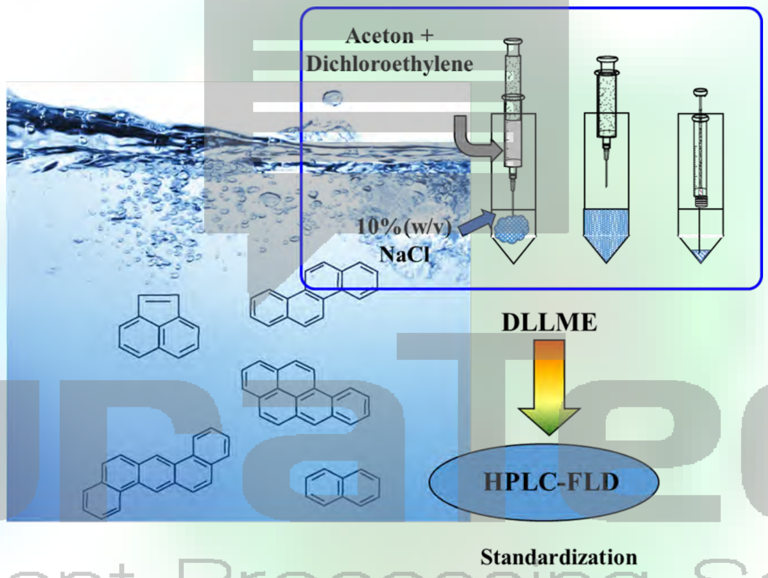
Graphical Abstract



Abstract: In this study, Dispersive liquid-liquid microextraction (DLLME) combined with High performance liquid chromatography-Multichannel Fluorescence detector (HPLC-FLD) as a simple, fast and inexpensive method have been optimized in order to develop a standard method for determination of polycyclic aromatic hydrocarbons (PAHs) in water samples. In the optimum condition, 6mL of extraction mixture contains aceton (disperser solvet) and dichloroethylene (extractor solvent) (50:1) are rapidly injected into the sample (30.00 mL) containing 1 mL of NaCl solution (10 w/v%). Therefore, a cloudy solution is formed. After centrifuging, the sedimented phase were transferred into a vial and evaporated at

35°C under nitrogen atmosphere. Thereafter, 200 μL acetonitrile is added to the vial, the obtained solution evaluated using HPLC-FLD. Under the optimum condition, it was possible to measure 14 PAHs compounds. The linear ranges for most compounds are in the range 0.5-0.5 μgL^{-1}.The recovery rate is between 65% -94% and the quantitative detection limit (LOQ) is in the range of 0.003-0.12 μgL^{-1}. The relative standard deviation (RSD%) in the concentration of 0.7 μgL^{-1} of PAHs were 4.5-7.7% (n=3). The method was validated by simultaneous testing of a spiked sample with the standard method (ISIRI 9387-2) and the mean results were compared using t-test. The extraction method was also coupled with gas chromatography-Mass spectrometer (GC-MS) to evaluate its performance and robustness. Finally, the optimized method was used to measure the concentration levels of PAHs in 40 water samples. The proposed procedure is can be developed to determine PAHs in other matrices. In order to standardization the method, its precision including repeatability and reproducibility, accuracy and robustness were tested.

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Antiviral Activity of Au-Doped Ag NPs Against Herpes Simplex Virus (In Vitro Study)

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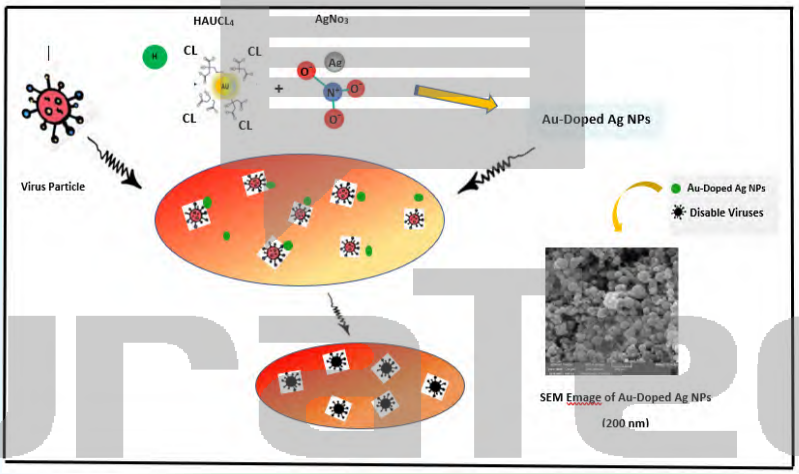

Abstrac: Viruses represent one of the leading causes of disease and death worldwide. Viral and Bacterial contamination of touch surfaces allows for transmission of pathogens leading to increased risk of infection. Virus infections pose significant global health challenges, In the present, nanoscale materials have emerged as novel antiviral agents for the possibilities offered by their unique chemical and physical properties. viruses spread through direct person-to-person contact and/or indirect contact via virus-containing airborne droplets or contaminated surfaces of objects such as floors, handrails, touch panel/buttons, or furniture.[1] Therefore, antiviral chemicals and/or materials are useful for protecting against the spread of pandemic-scale viruses. These

chemicals deactivate viruses by denaturising their proteins.[2] Here, we report a series of nanoparticles for antiviral activity using the herpes simplex virus type 1. We have identified Au-Doped Ag Nanoparticles as a material with the effec antiviral activity which retains its antiviral activity in liquid form and can therefore be widely used to minimize contamination and microbial transmission. The synthesized nanoparticles was characterized by powder X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FT-IR). According to the scanning electron microscope analysis of Au-Doped Ag Nanoparticles, the average particle size of the was 47.5 nm on the surface. The virucidal efficacy of Au-Doped Ag nanoparticles was investigated against the Herpes Simplex Virus type 1 (HSV-1) as a model; under the specific experimental and multiple time conditions. The antiviral effects of Au-Ag nanoparticles for blocking viral entry activity demonstrated an approximately 3-log reduction in a virus titer-based log reduction.

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Magnetically Recoverable Vanadium Catalysts for O-Acetylation of Alcoholes Under Solvent-Free Conditions

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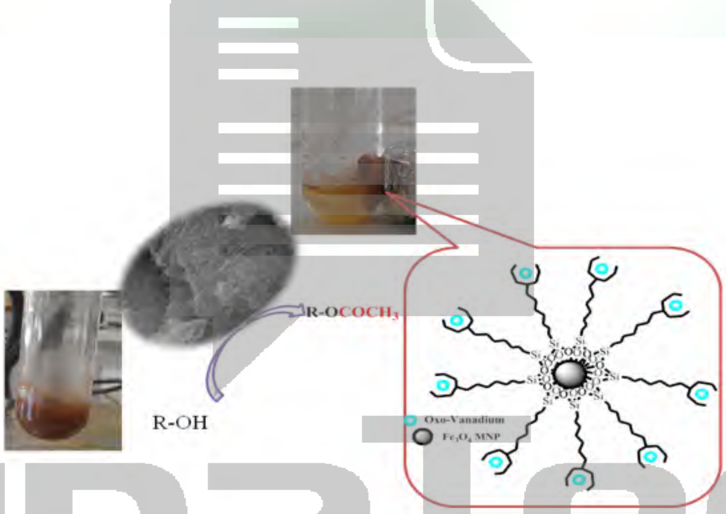

Abstract: The expansion of catalytic methods is a focus of contemporary interest due to the adverse effects of the manufacturing process of fine chemicals, pharmaceuticals, and materials on the environment. According to the green chemistry principles [1], the "green" catalyst is the one that can be simply removed from the reaction mixture and reused. In this field, magnetic nanoparticles have been the focus of great attention as a magnetically separable matrix for catalysts [2].

Also, it is clear that green chemistry not only requires the use of "green" catalyst but also development of solvent-free reactions is one of the most important research threads in green chemistry .Solvent-free conditions have advantages, such as simple reactors, easy work-up procedures, short reaction times and environmentally benignancy [3, 4].

The present paper explains that this approach allowed us to prepare the most active heterogeneous vanadium catalysts for the selective acetylation of alcohols .The paper also addresses a few important and interesting aspects of the catalytic reaction such as activity and selectivity for various substituents at the alcohols; also, recovery and reuse of the catalyst.

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Copper (II)- Supported on Fe_3O_4 Nanoparticles: Magnetically Recoverable and Reusable Catalyst for The Synthesis of Polyhydroquinolines

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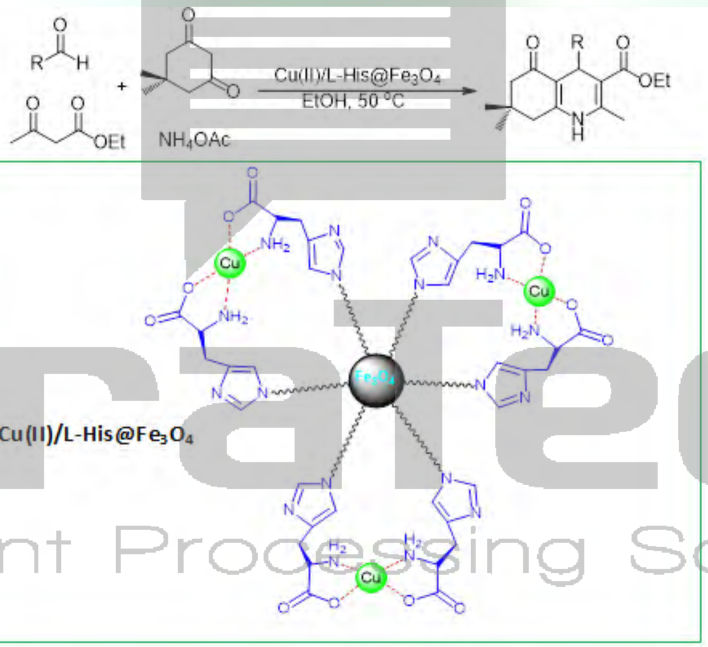

Abstract: Catalysis plays a dynamic role in achieving chemical conversions in an economically and commercially viable manner and is the foundational pillar of green chemistry as it offers a clear opportunity to provide realistic solutions to many environmental issues. In the present era, when pollution is a major problem, the focus is also on placing precincts to the use of conventional, corrosive and non-recoverable homogeneous catalysts and identifying robust, easy to handle, and recoverable heterogeneous catalysts. In recent years, magnetic nanoparticles have attracted much

attention because of their unique magnetic properties and widespread application in different fields such as mineral separation, magnetic storage devices, catalysis, magnetic refrigeration system, heat transfer application in drug delivery system, magnetic resonance imaging (MRI), cancer therapy, and magnetic cell separation [1–3]. The application of magnetite in the field of waste water treatment is becoming an interesting area of research [4]. Here we prepared a nanocatalyst by immobilization of the Cu(II)-L-Histidine complex on magnetic Fe_3O_4 nanoparticles. Copper (II) bound to L-histidine is in equilibrium with human serum albumin and may undergo common exchange which modulates the bioavailability of copper to the cell. Cu(II)/L-His@Fe_3O_4 as a novel, efficient and green nanocatalyst was applied successfully in the synthesis of heterocyclic compounds. The resulted catalyst was used in the synthesis of polyhydroquinolines as biologically interesting compounds, polyhydroquinolines exhibit a wide range of biological activities, such as antitumor, antibiotic, antipyretic, analgesic, antihypertonic and vasodilating behavior [5]. The protocol proves to be efficient and versatile benign in terms of very easy work-up and reused seven times without significant loss of catalytic activity.

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Preparation of New Alternative Transfer Sites by Combining MIL-53(Fe)-$(COOH)_2$ in Sulfonated Polystyrene/Polyethylene Membrane

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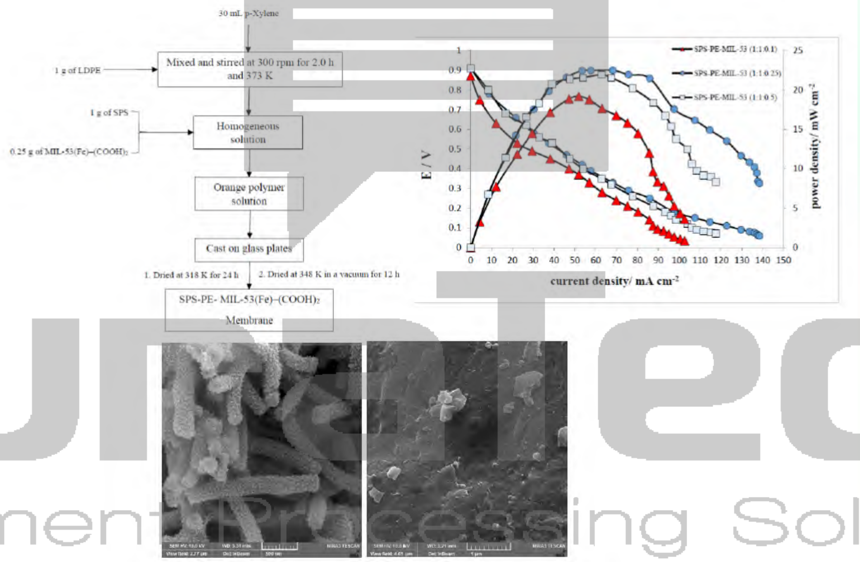
Graphical Abstract



Abstract: In this study, we prepared a novel proton exchanger membrane based on sulfonated polystyrene modification with MIL-53(Fe)-$(COOH)_2$ for application in direct methanol fuel cell. In these membranes, different amount of MIL-53(Fe)-$(COOH)_2$ were used to prepare the membranes. The membrane is characterized by FT-IR, SEM and TGA. Water uptake, proton conductivity, oxidative resistance, ionic conductivity and methanol permeability are measured to evaluate its performance in a direct methanol fuel cell with cation exchanger membrane. The SPS-PE-MIL-53 (1:1:0.25 w:w:w) membrane showed relatively better performance than the other

membranesThe prepared membranes were used in a fuel cell to evaluate the performance. All membranes prepared, in the fuel cell performed well, but the SPS-PE-MIL-53 (1:1:0.25 w:w:w) membrane performed better than other membranes. The DMFC based on SPS-PE-MIL-53 (1:1:0.25 w:w:w) membrane has a maximum peak power density of 22.49 mWcm^{-2} with maximum current density of 138.46 mAcm^{-2}. In general, the prepared membranes performed well than similar membranes.

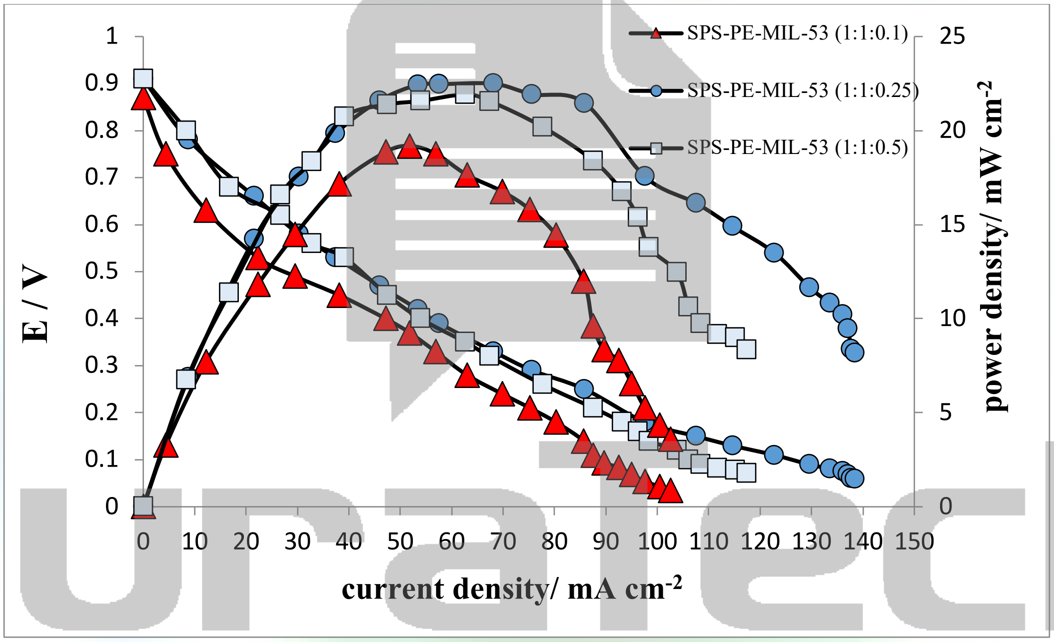


Fig. 1 Current density-potential (I-V) and power density curves of the DMFC assembled with different prepared membranes at 80 ºC.

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Treatment of Oily Wastewater Using Chemical/Biological Processes

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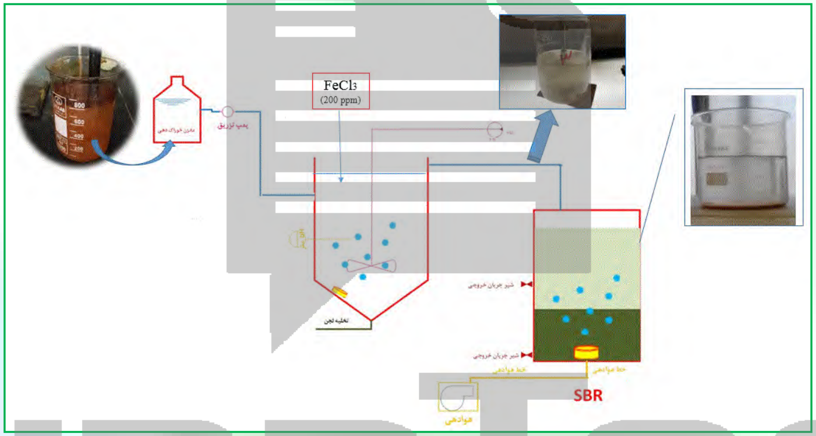
Graphical Abstract



Abstract: The importance of oil and natural gas in human life is clear. Water produced along with crude oil and natural gas (produced water) during the extraction of oil and gas wells; is the largest volume of produced wastewater in the oil and gas industry. More than 80% of the wastewater generated from the oil production process is produced water (PW). PW is a mixture of different organic and inorganic substances. Since water scarcity is one of the serious problems in the country, water and wastewater treatment is very important. In this study, a combination of chemical and biological processes was used to recover water associated with the production of oil and gas fields for industrial use. Because of the environmental standard, the chemical oxygen demand (COD) is very important; the COD parameter was used to measure the amount of wastewater treatment. Turbidity and residual Oil & Grease content were also analyzed. The initial

values of COD, turbidity, and oil & grease in the wastewater were 3350 mg/L, 25 NTU and 722 mg/L, respectively. In the chemical process, ferric chloride ($FeCl_3$) and poly aluminum chloride (PAC) coagulants were used and the results showed that the $FeCl_3$ coagulant had a higher efficiency with COD, turbidity and O&G removal rates of about 45%, 80%, and 90%, respectively. In the biological process, extracted and cultured oily-salt-loving microorganisms. Then, the sequential batch reactor (SBR) method was used, and the combined purification system over a period of 24 hr. resulted in a removal efficiency of about 85% for COD, 90% for turbidity and the amount of Oil & Grease was trace. Consequently, with chemical and biological combined methods can treatment the produced water wastewater and reduce the amount of organic load for reuse in the industry.

Keywords: Oily wastewater, Produced Water, Treatment, Chemical, Biological, SBR

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Ultrafine Polyamide-6 Nanofiber/Nets Membrane for Effective Air Filtration

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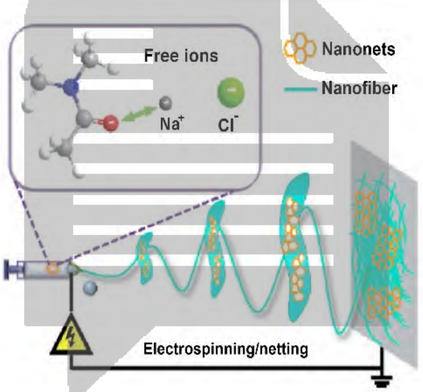
Graphical Abstract



Abstract: Particulate matter and spread of COVID-19 caused by SARS-CoV-2 are two of the most serious problems because of their significant threat to human health .Ultrafine and bimodal structured polyamide-6 nanofiber/nets (PA-6 NFN) membrane via one-step electrospinning/netting.The PA-6 NFN membranes are combined of ultrafine (~70 nm) nanofibers and covered two-dimensional (2D) ultrathin (~20 nm) nanonets which are optimized by facilely regulating the solution concentration, ionization of the solution by adding NaCl and applying a high voltage of 22 kV are effective in forming this specific structure. With integrated properties of small pore size, high porosity, and high specific surface area, the resulting PA-6 NFN membranes exhibit robust mechanical strength of 12.32 MPa, high filtration efficiency of 99.11% for the 100 nm aerosol particles, low pressure drop of 81Pa, higher quality factor compared to two standard commercial masks including Three-Ply surgical mask and respirator face mask, combined with large particle holding capacity of 108 g/m^2 and ability to maintain conditions 5 filtration cycles for filtrating ultrafine airborne particles. The diameter of the SARS-CoV-2 ranged from 60 to 140 nm is considered, therefore PA-6 NFN membranes could preventing dispersal of droplets and reduce the spread of COVID-19 caused by SARS-CoV-2. In addition, the filtration efficiency calculation results show that the good agreement with the measurement results. The fabrication of PA-6 NFN medium makes it a promising candidate for $PM_{0.3}$ governance at applications including face mask, protective clothing, clean room and engine intake.

Keywords: Nano fibers;air filtration; SARS-CoV-2; Filtration fabrics; Engineered textiles; Technical textiles

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Ionic Liquid-Derived Magnetic Mesoporous Carbon as A New Magnetic Sorbent for Dolid-Phase Extraction of Triazine Herbicides in Water Samples

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Abstract: Triazine herbicides are one of the most widely used herbicides and have caused much concern about their toxic effects on human and ecosystem. Their wide application may cause pollution to soil, crops, surface water and other drinking water sources due to their large dosage, stable chemical property, long residue time and higher water solubility [1-2]. In the present work, a new and efficient method for ultra-trace determination of triazine herbicides in water was developed, using magnetic mesoporous carbon-based solid-phase extraction, followed by high performance liquid chromatography determination. The sorbent was synthesized using an imidazolium-based ionic liquid as the carbon source, guanine as the nitrogen source, $FeCl_3$ as the iron source, and SBA-15 as the hard template. The effects of sample pH, extraction time, type and volume of elution solvent and extraction solvent, desorption time, and salt addition on the extraction efficiency of atrazine were examined and optimized. Under the optimum conditions, the LODs, LOQs, and, LDR were in the range of 0.08–0.34 ng mL^{-1} and 0.25–1.14 ng mL^{-1}, 0.25-100 ng mL^{-1}, respectively. The developed method was applied to the determination of triazine herbicides in river and lake samples, with RSD of 2.9–10.5%. Therefore, the proposed method allows proper monitoring of trace triazine herbicides in various environmental waters.

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Quantification of Chromium Species by Gel-Electro-Membrane Extraction as A Green Method in Environmental Samples

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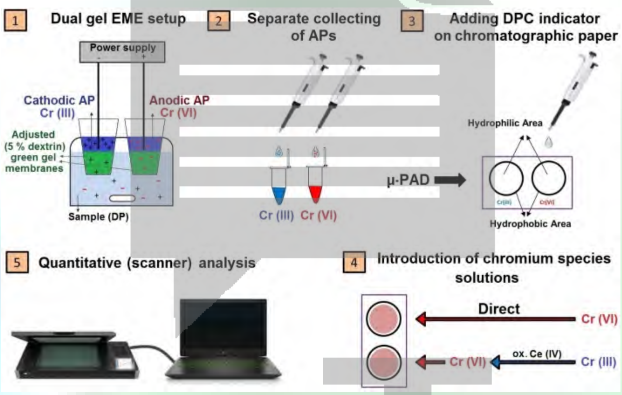
Graphical Abstract



Abstract: For the first time, gel-electro-membrane extraction (G-EME) as a green extraction method was used to determine Cr(III) and Cr(VI) in environmental samples. In this regard, various agarose-based gel membrane types with low-, medium- and high-EEO were fabricated and tested. Cr(III) and Cr(VI) were simultaneously extracted from an aqueous sample (pH 3.0) *via* the cathodic and anodic gel membranes (pH 3.0 for both membranes), into the cathodic and anodic aqueous acceptors (200 µL each, pH 2.0), respectively. After extraction at the optimal conditions (i.e., voltage: 32 V, extraction time: 22 min), the both compounds were quantified by a cheap and easy-to-perform reader platform termed as microfluidic paper-based analytical device (µPAD). The anodic acceptor phase containing Cr(VI) was analyzed directly by µPAD (after adding diphenylcarbazide – DPC – as a selective colorimetric reagent, to the detection zone). The cathodic acceptor phase containing Cr(III) was mixed with Ce(IV) to oxidize Cr(III) → Cr(VI). Cr(VI) ions were then analyzed again by µPAD after adding DPC. ImageJ software was used for the quantitative analysis of µPAD scans based on measuring the intensity of the violet color. The results showed that high extraction recoveries referred to 87% for Cr(III) and 75% for Cr(VI), were acquired when the low-EEO agarose gel membrane with 5% (w/v) dextrin was used. Also, limits of detection (LODs) of 0.5 and 0.7 ng mL^{-1} for Cr(III) and Cr(VI) were obtained, respectively.

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Introduction of Nitrogen Doped Graphene Nanosheets as Efficient Adsorbents for Nitrate Removal from Aqueous Samples

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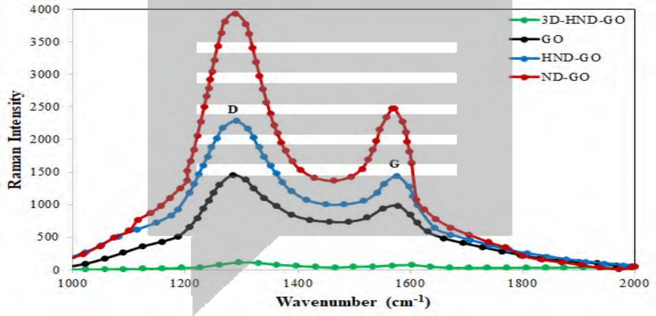
Graphical Abstract



Abstract: Introducing and developing new kinds of adsorbents are always a significant challenge in water treatments. In this work, for the first time, graphene oxide (GO), nitrogen-doped graphene oxide (ND-GO), highly nitrogen-doped graphene oxide (HND-GO), and 3D high nitrogen-doped graphene oxide (3D-HND-GO) were synthesized and comparatively evaluated in the removal of nitrate content of tap and underground waters. Based on the results, 3D-HND-GO showed the highest removal efficiency in comparison with the other mentioned nanoparticles. In addition, the optimal removal condition was achieved using the Nelder-Mead non-linear optimization algorithm as follow: the initial concentrations of nitrate (expressed as nitrogen): 15.0 mg/mL, the amount of the adsorbent: 2.0 mg/mL; pH of the sample: 3.0; and the contact time: 20.0 min. Under this optimal condition, the actual removal result (92.5 ± 4.0%) was in good agreement with the expected value (94.8 ± 5.1%). The adsorption isotherm complied with the Langmuir model illustrating the considerable mono-layer adsorption capacities for the target ions with q_m of 8.7 mg/g. This study revealed which 3D-HND-G leads to improved yield in the nitrate ions elimination, particularly at acidic media, which was related to the enhanced dispersibility and larger surface area. The adsorbent was further successfully used for treating tap and underground water samples. At the present moment, research as grown to modify 3D-HND-G in orders to increase the potentiality for industrial applications.

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Methyl orange-Functionalized Silver Nanoparticles as A Probe for Fluorometeric Determination of Arsenic (III) in Water Samples

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Abstract: Arsenic (As) is a high toxic element found in food and drinking water [1]. Among various arsenic species, As (III) and As (V) are the most important species in natural waters and its direct exposure is harmful to humans due to its carcinogenic effects on the hematopoietic system, liver, , and central nervous system. According to the World Health Organization (WHO) and the U. S. Environmental Protection Agency(EPA),the maximum permissible limit for arsenic in drinking water is as low as 10 μg L^{-1} [2]. Therefore, development of a simple, fast, inexpensive and sensitive analytical procedure for the determination and monitoring of trace level of arsenic contamination in different samples such as water, food and plants is of great importance. Different analytical procedure have been employed for arsenic determination, of which the most important are atomic absorption spectrometry, atomic fluorescence spectrometry, UV–Vis spectrophotometry, inductively coupled plasma along with optical emission spectrometry or mass spectrometry, cathodic stripping voltammetry and polarography [3]. In this work a simple, sensitive and rapid fluorometeric method for determination of As (III) was developed using methyl orange-functionalized silver nanoparticles. By increasing the concentration of arsenic, the fluorescence intensity was increased. The parameters affecting the fluorescence intensity such as pH, temperature and reaction time were optimized. Under the optimum conditions, the calibration

graph was linear over the range of 100-200 μg L^{-1}. The relative standard deviation (R.S.D., n = 5) was lower than 3%. The method was successfully applied to the determination of trace amount of As (III) in water samples.

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Extraction of Diazinon and Chlorpyrifos Pesticides in Some Vegetables Using Magnetic@Chitosan@SNW-1 Followed with QECHERS Method

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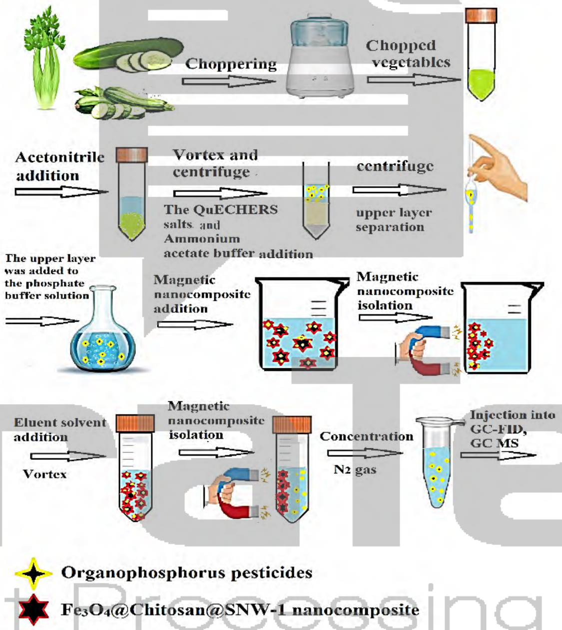
Graphical Abstract



Abstract: Extra residual amounts of organophosphorus pesticides (OPPs) in the body of the living organisms hve toxic effect on the central nervous system which can lead to paralysis, suffocation, or even death. Maximum residue levels (mg kg^{-1}) of diazinon and chlorpyrifos in the Cucumber, Celery, and Zucchini vegetables are 0.01 mg kg^{-1}. Therefore, measurement of in OPPs in agriculture samples is essential. High porosity and specific surface area of covalent organic frameworks (COFs) make them suitable compounds in extraction of the analytes. Also schiff base network-1 (SNW-1) can make interactions with various analytes by H – bonding interaction, π-π interaction with nitrogen atoms and Pi. On the other hand, there are amines and hydroxyl groups in the linear structure of chitosan (CS) which cause this biopolymer to make suitable interactions with various molecules. In this method, a novel and green magnetic nanocomposite (M-CS-SNW-

1 nanocomposite) was synthesized and used for extraction and preconcentration of diazinon and chlorpyrifos pesticides from the vegetable samples. The QuEChERS method was applied for clean-up and simplify the complex matrix of the real examples before analysis. Separation and determination of pesticides were done by GC-FID and GC-MS instruments. The optimization parameters such as pH, sorbent amount, adsorption time, desorption type, desorption time, desorption eluent, eluent volume, and sample volume were investigated. Under optimum conditions analytical parameters of the method including limit of detection = 0.008 and 0.01 µg L^{-1}, linear range = 0.04 -500 and 0.07 -500 µg L^{-1}, relative standard deviation (C = 80 µg L^{-1}, n = 4) = 2.3 and 4.7, and enrichment factor = 65 and 283 were obtained for diazinon and chlorpyrifos, respectively. The relative recoveriesin real samples confirm the efficiency of the present method for determination of OPPs pesticides in vegetable samples.

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The Effect of Structure and Form of TiO_2 Photocatalyst on The Methylene Blue Degradation from The Wastewater

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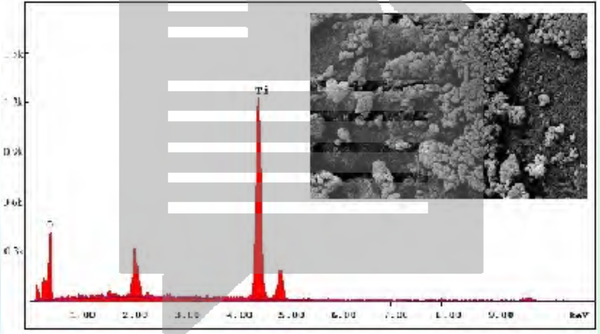
Graphical Abstract



Abstract: Semiconductor photocatalyst reduction has been a new considerable technology for the removal of various toxic pollutants such as dissolved heavy metals and organic materials. Titanium dioxide with different forms is well-known as an excellent photocatalyst among the photocatalyst semiconductors for the wastewater treatment. In this work, firstly, TiO_2 was prepared in anatase and rutile forms by sol-gel methods. Then, the photocatalytic properties of anastase nanoparticles was evaluated using XRD, FT-IR, FESEM-EDX, and BET methods. The most important variables including methylene blue dye concentration, TiO_2 nanoparticle dosage and pH under UVA light irradiation in 90 min were examined to obtain the optimum conditions for the photocatalytic process. Also, the photocatalytic efficiency of anatase, rutile, and commercial TiO_2 was compared together for photodegradation of methylene blue. The absorbance peaks of FT-IR determined Ti-O-Ti bond and located in the type IV related to mesopor structure corresponding to IUPAC classification. The result of FESEM indicated the almost spherical shape and existence of Ti and O in the particles which are pure. The maximum photocatalytic efficiency of the as-prepared nanoparticle in methylene blue removal was about 70% under the optimized parameters including photocatalyst dose of 0.3 g/L, pH ≈11, temperature ≈30 °C and dye concentration of 10 mg/L after 90 minutes UVA irradation. The compression among anatase, rutile, and commercial TiO_2 showed removal amount of anatase is more than rutile for reducing the mesoporous structure in high

activation temperature. Therefore, the experimental data showed that the as- synthesized photocatalst is able for industrial wastewater treatment.

Keywords: photodegradation, anatas, rutile, mesopour.

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A High Yield Synthesis Fe_3O_4/TiO_2/GQDs Nanocomposite for Photodegradation of Imipramine from Wastewater

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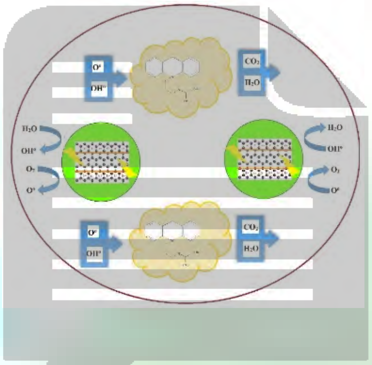
Graphical Abstract



Abstract: The pharmaceutical wastewater includes significant amounts of toxic pollutants that needs to treatm ent by using advanced methods. In this study, the photocatalytic degradation of imipramine in aquatic media was investigated by the prepared photocatalyst magnetite titanium dioxide loaded by graphene quantum dots (Fe_3O_4/TiO_2/GQDs). Firstly, photocatalyst Fe_3O_4/TiO_2/GQDs synthesized in four steps which included co-precipitation, sol-gel, and hydrothermal methods for preparation of Fe_3O_4, TiO_2, GQDs, and nanocomposite, respectively. Then, the morphological, and structural properties and quality of the nanocomposite were investigated using different methods comprising XRD, SEM, BET, and TEM. Finally, the efficiency of photocatalytic degradation was examined to obtain optimum parameters that effected on pgotocatalyst application. The diffraction peaks of XRD data were accordance with the Fe as magnetite, Ti as anatase and graphene quantum dots formation. SEM and TEM analysis of the prepared nanocomposite indicated the spherical and size of particles. BET results showed mesoporous structure with desired characteristic. Then, the effect of different variables showed photocatalyst dose of 0.5 g/l, pH ≈3, temperature ≈40 °C for 120 minutes under UVA irradiation source (9W) were optimized condition. The maximum removal efficiency from real effluent was about 70% in optimum. Also, the results obtained the major degradation mechanism of imipramine was direct oxidative decomposition through the photogenerated holes. The kinetic study of reactions indicated, the photocatalytic decomposition of imipramine followed by the apparent first-order models under the UVA light irradiation. The results show the synthesized photocatalysts Fe_3O_4/TiO_2/GQDs can be applied in the treatment of industrial effluents containing persistence organic pollutants under optimal conditions.

Keywords: Fe_3O_4/TiO_2/GQDs, photocatalytic process ;imipramine.

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Using Micro-Extraction on A Screw for Determination of Trace Amounts of Cationic Dyes by HPLC-UV/Vis.

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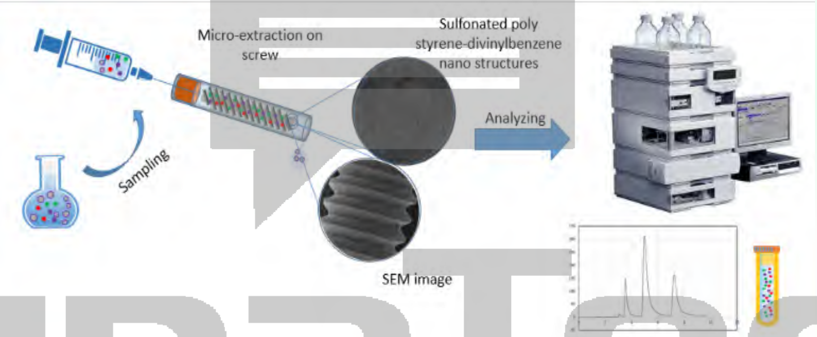
Graphical Abstract



Abstract: Nowadays, among all pollutants, cationic dyes are one of the biggest concerns in contemporary society. These dyes pose a serious threat to human health and the environment due to their toxic, non-biodegradable, and even carcinogenic effects. Therefore, it is important to develop sensitive techniques for determining these colors in real samples [1].

In general, sample preparation is an important step in separation techniques and accurate determination of the desired analyte from complex matrices [2]. Among the sample preparation methods, solid phase micro-extraction (SPME) is more popular. SPME is found useful for micro-extraction due to its small geometry and simple operating procedures, simplicity, rapidity, accurate analysis and low consumption of organic solvent [3].

In the present work, solid phase micro-extraction on a screw (MES) which is a miniaturized form of in-tube SPME without back pressure, was developed to extract cationic dyes (malachite green,

methylene blue and rhodamine B) in water samples. The screw was coated with a functionalized co-polymer as an absorbent. The extracted dyes on the screw was eluted by a suitable eluent. Separation and determination of the dyes was performed by high performance liquid chromatography equipped with a UV detection (HPLC-UV). Hence, MES is prepared by electrophoretic coating sulfonated poly (styrene-co-divinylebenzene) on surface of a screw. Then it was placed inside a silicon tube to create a channel to pass sample solution through it. Effective parameters on extraction efficiency of analytes were studied and optimized. Under optimum conditions, the limit of detection was 0.15 µg L^{-1} and calibration curve was liner in the range of 0.5-250 µg L^{-1} with a correlation coefficient greater than 0.98 for all studied cationic dyes. The inter-day and intra-day precision (n=5) were 2.8-7% and 7-9.5%, respectively. The proposed method is evaluated as a simple and repeatable method with acceptable relative recoveries (82-103%) for determination of cationic dyes in real water samples.

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Filter Paper Modified with Polyaniline as A Sorbent for Solid-Phase Microextraction of Cadmium Ions

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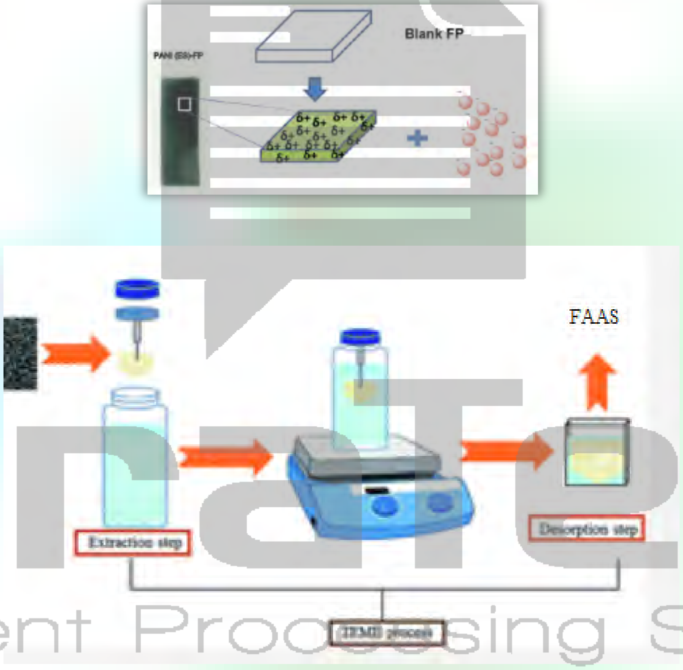
Graphical Abstract



Abstract: Trace levels of heavy metals are widely spread out in the environment due to industrial and agricultural processes. The monitoring of these elements in a great variety of environmental and biological samples is required because of their toxicity. Cadmium is one of the most known hazardous elements to human health which accumulates in the body mainly in the Kidneys and Liver. Direct determination of a low level of cadmium with the well-available technique of flame atomic absorption spectroscopy is not possible due to the complexity of the environmental sample

as well as the limitation of the instrument detection limit. Thus, a separation and preconcentration step before its determination is required. Among various microextraction methods reported for the separation and preconcentration of cadmium ions, solid-phase microextraction (SPME) has the advantages of reduction of analyzing time, use of less amount of solvent, high preconcentration factor, ease of manipulation, and simplicity of automation [1-2]. In this study, a new, environmentally friendly sorbent based on biopolymer was fabricated and applied for thin-film microextraction (TFME) of cadmium ions from various matrices. Filter paper which is mostly composed of cellulose, a biodegradable polymer, was modified by polyaniline [3]. The resulting positively charged modified filter paper was used as the sorbent in TFME of cadmium ions as its anionic complex of CdI_4^{-2}. The sorbed analyte was eluted from the sorbent by 0.5 mL of sodium hydroxide (0.5 mol L^{-1}) and quantified by flame atomic absorption spectrometry. Factors influencing the sorption and desorption of the anionic complex of cadmium were investigated and optimized. Under the optimized conditions, the method exhibited a linear dynamic range of 0.25-25 μg L^{-1}, a detection limit of 0.06 μg L^{-1}, and an enrichment factor of 200. The relative standard deviation for the determination of cadmium ions (n = 6) at 3 μg L^{-1} was 3.4%. The proposed method was successfully applied to the determination of cadmium ions in various environmental water samples.

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Electromembrane Microextraction Combined with Slug Flow Microextraction for The Analysis of Narcotics in The Wastewater Samples Followed by Ion Mobility Spectrometry

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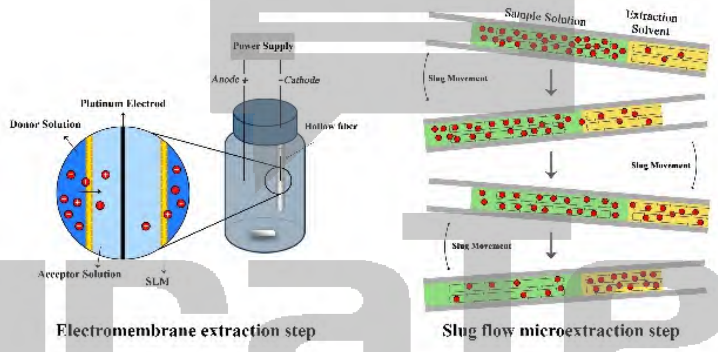
Graphical Abstract



Abstract: Narcotic drugs in general have been prescribed for their painkiller effects and are known to be the most widely used analgesics for the treatment and management of moderate to intense pains. The evaluation of the concentration of these substances in biological samples is extremely essential as an aid for efficient control of medical treatment, detection of narcotic doping and abuse prevention [1-3]. This study exhibits for the first time a combination of the electromembrane extraction (EME) with the corona discharge ion mobility spectrometry (CD-IMS) using the slug flow microextraction (SFME) between them as a useful tandem microextraction procedure. Following the workflow, at the first step (EME), target analytes were extracted from the donor

phase (DP) into the acceptor phase (AP) utilizing an electrical field. After that, the AP was collected and its pH was adjusted to be used as a DP in the subsequent step (SFME). Then, the SFME method was performed at appropriate conditions and analytes migrated to the organic solvent. Finally, the organic solvent was collected and used for the determination of narcotics by CD-IMS. This coupled method was utilized to quantify narcotics (methamphetamine, methadone, tramadol, and buprenorphine) in the wastewater samples. Box-Behnken design (BBD) and the response surface methodology (RSM) were employed for the optimization of effective factors on the extraction efficiency. Under the optimized extraction condition, good linearity was obtained in the range of 0.5-750 ng/mL with coefficients of determination ≥ 0.991. The limit of detection and quantification were achieved in the range of 0.15–0.2 ng/mL and 0.5–0.75 ng/mL, respectively. The inter-day and intra-day precisions were not exceeding 11.5%. Also, using EME-SFME/CD-IMS system causes the enrichment factors to rise up to 2.7 times and the limit of detection (LOD) to decrease to 15 times, compared to the EME/HPLC-UV. Finally, 50 ng/mL and 250 ng/mL of each narcotic were spiked into the wastewater samples.

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One-Pot, Four-Component Domino Synthesis of Bis-Benzo[*c*]Pyrano[3,2-*a*]Phenazine Derivatives Using New Complex of 2-Amino-1H-Purin-6(9H)-One Supported Into MCM-41 Mesoporous

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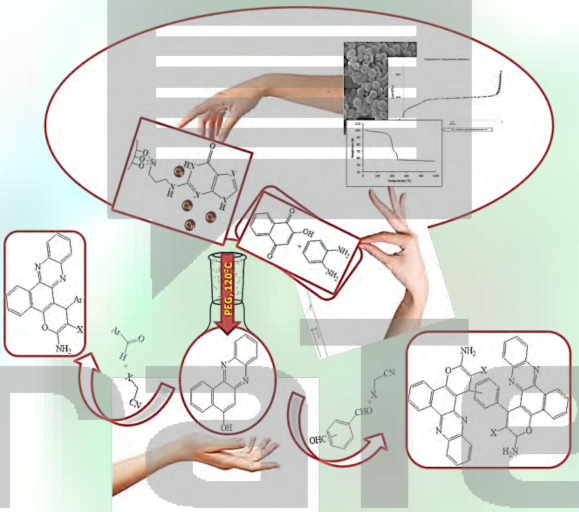
Graphical Abstract



Abstract: A new one-pot, two-step, four-component synthesis of bis-benzo[*c*]pyrano[3,2-*a*]phenazine derivatives were carried out by reaction of 2-hydroxy-1,4-naphthoquinone, benzene-1,2-diamine, carbonyl compounds and alkylmalonates using new cupper (II) ions complex of guanine (2-amino-1H-purin-6(9H)-one) supported into MCM-41 (Cu-guanine-MCM-41) channels as efficient and heterogeneous catalyst in PEG. The desire products were obtained in good to excellent yields. The prepared catalyst can be reused for several times without any significant loss of its catalytic activity.

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Zirconium Oxide@2-amino-1H-purin-6(9H)-one@MCM-41: A Stable and Efficient Heterogeneous Catalyst for One-pot, Four-component Domino Synthesis of Benzo[a]benzo[6,7]chromeno[2,3-c]phenazine and Spiro[benzo[a]benzo[6,7]chromeno[2,3-c] phenazine] Derivatives

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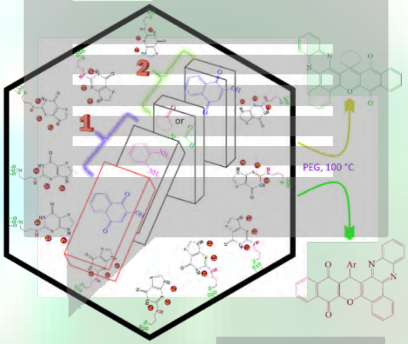
Graphical Abstract



Abstract: MCM-41-supported nanoscale guanine bonded with Zr(IV) was prepared using sol-gel method and characterized by SEM, BET, XRD, TGA, TEM, Raman and FT-IR spectroscopy. This compound was employed as an efficient heterogeneous catalyst for preparation a series of benzo[a]benzo[6,7]chromeno[2,3-c]phenazine and spiro[benzo[a]benzo[6,7]chromeno[2,3-c] phenazine] derivatives by one-pot, four-component domino reaction from the 2-hydroxy-1,4-naphthoquinone, benzene-1,2-diamines, 2-hydroxy-1,4-naphthoquinone and carbonyl compounds in PEG, at 100°C. The Zr-gu-MCM-41 can be recycled four runs without any significant loss of its catalytic activity.

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Indirect Electrochemical Oxidation of Amines using Triazolinediones as an Environmentally Friendly Method

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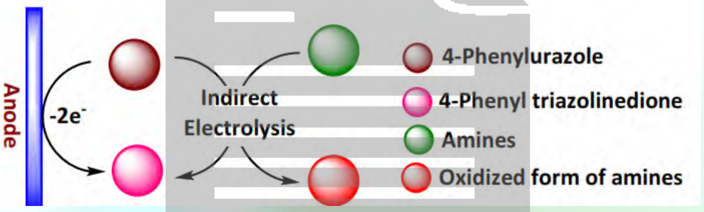
Graphical Abstract



Abstract: Organic electrosynthesis is one of the promising methodologies by having important criteria which is needed if society is to develop environmentally compatible processes. Eliminating toxic or hazardous oxidizing or reducing reagents, economical energy consumption, and *in situ* production of unstable and dangerous reagents are some advantages of this strategy. Electrosynthesis covers at least nine priciples of twelve green chemistry principles. Among electrochemical procedure "indirect electrolysis" provides an important option to create catalytic synthetic processes with decreased energy consumption and chemical waste. The catalyst is regenerated at the electrode and only small quantities of the redox reagent are used. Electrochemical oxidation of amines has a great attention due to industrial importance. Amines participate in many important biological and chemical reactions and hence are of interest in the food, corrosion, agrochemicals, pharmaceutical, and other industries. Herein we introduce triazolinediones as perfect mediatior for efficient amine oxidation. The oxidized form of 4-phenylurazole (4-phenyl triazolinediones) is highly unstable and ring cleavage occurs due to the simultaneous presence of both carbonyl and azo moieties. Instability is more critical by the

presence of electron-withdrawing group in the structure. However, the results reveal triazolinediones promote a wide range of amine oxidations despite high instability due to fast chemical kinetic of oxidative ring cleavage. The results of current work indicate that electrochemical oxidation of urazole in the presence of amine is not a simple electrocatalytic reaction (*EC′* (*E:* electron transfer, *C*': catalytic chemical reaction)). The voltammogram features show that reaction proceeds via both *EC′* and *ECE* pathways. However, the reactions are strongly influenced by media and reaction conditions. In this study, the effect of different parameters such as pH, concentration ratio of amine to urazole, substitute effect of triazolinedione and amine have been studied. Moreover, the effects of electronic and structure nature of amines were evaluated for aromatic, aliphatic and benzylic amines.

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Evaluation of Microbial Electro-Fenton System Performance in Removal of Tetracycline Antibiotic from Wastewater and Renewable Energy Generation Under the Influence of Different Electrical Circuit Conditions

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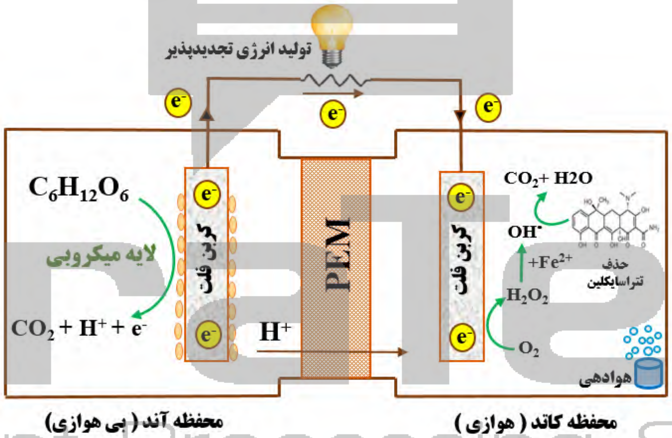
Graphical Abstract



Abstract: Microbial electro-Fenton system is a new and green technology that has the ability to remove resistant organic pollutants due to cathodic Fenton reactions along with the production of renewable electrical energy through the catabolic activity of microorganisms. The aim of this study was to evaluate the performance of microbial electro-Fenton system in tetracycline antibiotic removal as a target contaminant from wastewater and energy generation under the influence of different electrical circuit conditions. In this study, a two-chambered microbial electron-Fenton system equipped with anode and cathode electrodes made of carbon felt, Nafion membrane with 2000 mg/L substrate and anaerobic sludge as inoculum was operated in open, closed and short circuit conditions for 24 hours. During the operation of the reactor, the effect of the type of electrical circuit on the cathodic removal efficiency of tetracycline and the production of electrical energy was investigated. Electrical circuit conditions were introduced as important parameters in generating electricity and removing contaminants in the cathode. The findings of this study proved that the efficiency of the microbial electro-Fenton system in tetracycline removal in short circuit conditions due to increased production of hydrogen peroxide at the cathode, increased compared to open and closed circuit conditions and the removal efficiency of this pollutant in these conditions reached 99.04%. In addition, the current density generation in short circuit conditions improved compared to closed circuit conditions and the voltage of 260 mV, the power density of 93.13 mW/m^2 in the current density of 695 mA/m^2 were obtained in short circuit conditions. The results of this study showed that the microbial electro-Fenton system can be a suitable technology for clean and renewable electricity production and also simultaneous removal of various organic pollutants from the wastewater in different conditions of the electrical circuit.

Keywords: Microbial electro-Fenton, Tetracycline, renewable energy

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Graphene Oxide Doped Soluble Eggshell Membrane Composited to Fe_3O_4 Nanoparticles (GO/SEP/ Fe_3O_4) as An Efficient Nano-Sorbent for Removal of Tartrazine

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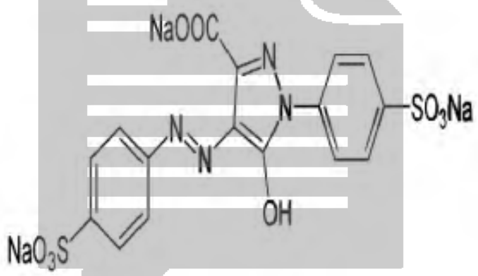
Graphical Abstract



Abstract: Graphene, a new class of 2D carbon nanomaterials with one atom thickness, has attracted considerable attention in recent years [1]. Eggshell membrane is a cheap, green and easily achievable biopolymer which have been used frequently in analytical science [2]. Tartrazine, a yellow menace, is widely being used in cosmetics, foodstuffs, medicinces and textile. It is carcinogenic and also catalyzes allerfic problems. In the present work the ability to remove Tartrazine from aqueous haz been studied using was material as adsorbent. Effects of pH, concentration of the dye, temperature and adsorbent doge have been studied. Results were analyzed by the Frundlich and Langmuir equation at different temperatures and determined the characteristic parameters of each adsorbtion isotherm. The adsorbtion process has been found thermodynamic parameters. Gibb's free energy ($\Delta G°$), change in enthalpy ($\Delta H°$) and change in entropy ($\Delta S°$) have been calculated. By rate expression and treatment of date in has been established that the adsorbtion of Tartrazine over han feathers follows a first - order kinetics and a film diffusion mechanism operaters at all the temperatures.

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Facilitated Transport of Bi(III) Through A Bulk Liquid Membrane with Aliquat 336 as A Carrier

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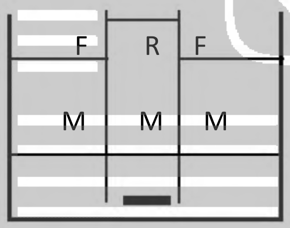
Graphical Abstract



Experimental set-up for the transport experiments: (F) feed phase, 10 mL; (M) liquid membrane, 20 mL; (R)receiving phase, 5mL.

Abstract: Bismuth is considered as an environmentally significant element, due to numerous applications of its compounds in different areas, which include: semiconductors, cosmetics and pharmaceuticals as well as chemical and metallurgical industries. Since the use of bismuth and its compounds in different areas of life has increased, toxicity of this element started to be considered for humans, animals and plants [1]. Various analytical techniques have been reported for the determination of Bi (III) in different samples. Flame atomic absorption spectrometry has the advantages of low cost and simplicity, but direct determination of bismuth is seldom carried out due to the relatively poor sensitivity. Therefore, a preconcentration procedure is often required to improve the detectability of FAAS [2]. The use of liquid membranes containing specific metal ion carriers offers for selective separation and concentration of the metal ions from aqueous solutions [3]. In this work Aliquat336 was used as a highly efficient carrier for the transport of bismuth ions through a chloroform bulk liquid membrane. The transport yield of bismuth ions (pH = 3) through a chloroform solution of Aliquat 336 (0.035 mol L^{-1}) into the receiving phase (sodium chloride 0.05 M) in the stirring rate 400 rpm was found to be 100± 2 % after 4 h. The selectivity and efficiency of bismuth transport from solution containing a competing ion was investigated. Results showed that the interfering effect of the various ions tested was negligible. Under the optimum conditions the limit of detection (LOD) and enhancement factor (EF) were 0.00303 ugL^{-1} and 147 respectively. This method was successfully applied to the determination of Bi (III) ions in waste water, samples.

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Platinum Nanoparticles Loaded on Nickel- and Nitrogen-doped Graphene Nanotubes Framework as A High Performance Electrode in Ethanol Oxidation Reaction

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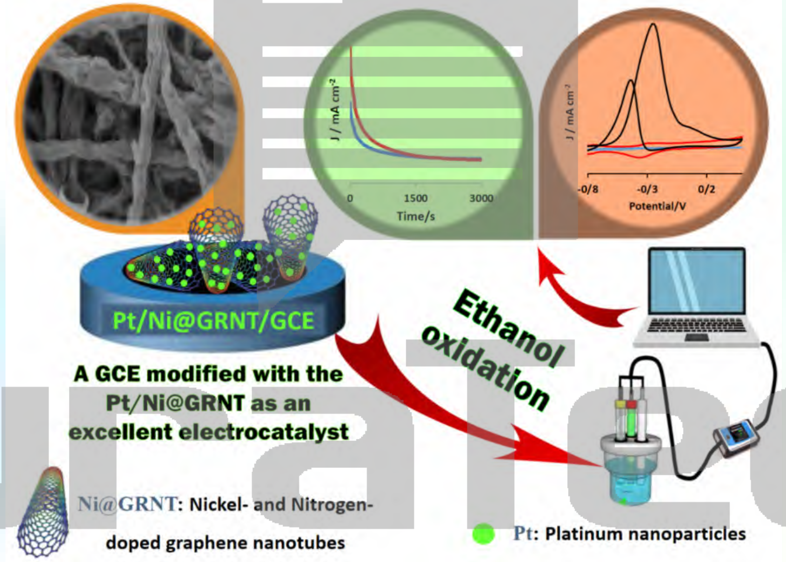
Graphical Abstract



Abstract: Ethanol is a perfect fuel in low-temperature fuel cells. Existing catalysts for ethanol oxidation in direct ethanol fuel cells are faced to considerable challenges thanks to their poor performance and CO like intermediates poisoning tolerance at anode surface. Therefore researchers are searching for new electrocatalysts within the the ethanol oxidation. During this study, Pt-loaded Ni-doped nitrogen-rich graphitic nanotube (Pt/Ni@GRNT) was synthesized employing a two-step procedure where the precursors were 1st refluxed to make a supramolecular assembly followed by a pyrolysis and leaching stage to form nanotubes. Thus, Pt was loaded on the outer surface of nanotube by an ultrasound assisted procedure. In order to confirm the right preparation of Pt/Ni@GRNT, it was characterized by FE-SEM, FT-IR spectroscopy and X-ray diffraction (XRD). Several electrochemical techniques like cyclic voltammetry (CV), and chronoamperometry (CA) were used to evaluate the oxidation of ethanol. Both CA and CV results highlight that Pt/Ni@GRNT exhibits improved electrocatalytic activity and stability towards ethanol oxidation. The Pt/Ni@GRNT electrocatalyst has excellent potential for application in ethanol fuel cells.

Keywords: platinum nanoparticles, graphene nanotubes, electrocatalyst, ethanol oxidation reaction.

Synthesis, Characterization, Optical Studies and Degradation of Organic Pollutant by Y_2O_3-coated Diatomite Modified with Zn^{2+}

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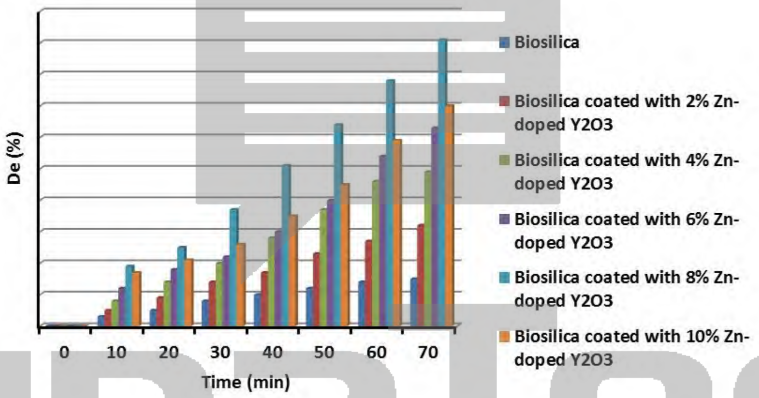
Graphical Abstract



Abstract: Degradation of hazardous organic contaminants in industrial wastewater through AOPs (advanced oxidation processes) has attracted a huge deal of research attention. Sonocatalysis is one type of AOP process that has recently been applied for degrading organic dyes . In this research, Zn-doped Y_2O_3 coated biosilica nanostructures with variable Zn^{2+} contents were synthesized by a facile hydrothermal technique. The products were characterized by means of energy dispersive X-ray photoelectron spectroscopy (EDX), scanning electron microscopy (SEM), X-ray diffraction (XRD), Brunauer-Emmett-Teller (BET), UV-Vis diffuse reflectance spectroscopy, and photoluminescence spectroscopy techniques. As claimed by XRD, the particles were crystallized excellently and attributed to the cubic phase of Y_2O_3. The cell parameters of the synthesized materials were calculated from the XRD patterns. With increasing dopant content (x),

a, b and c parameter for Zn^{2+} increases . High porosity and the surface morphology of diatom can be employed as the template to enhance potential of functional materials. The diameter of these particles in case of 8% Zn-doped Y_2O_3-coated with biosilica is around 20–65nm. . Changing the mass ratio of the substrate–diatomite and the coating material–doped-Y_2O_3 controls the thickness of the coating layers. The influence of substitution of Zn^{2+} ions into Y_2O_3 lattice caused a redshift in the absorbance and a decrease in the bandgap of as-prepared coated compounds. The pore volume and BET specific surface area of Zn-doped Y_2O_3 -coated diatomite is greater than uncoated biosilica. The photocatalytic activities of as-synthesized specimens were evaluated for the degradation of Reactive Red 43. The doped samples with proper content of Zn^{2+} ion had much better catalytic performance compared with uncoated biosilica. For diatom coated 8 % Zn-doped Y_2O_3 nanoparticles, the highest decolorization efficiency was achieved. The effect of various specifications like ultrasonic power, various scavenger, and catalyst amount was explored. The results revealed that diatomite coated with Zn^{2+}-incorporated yttrium oxide nanoparticles can be utilized in various experimental cycles with no significant drop in photocatalytic activity.

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Design and Fabrication of Optical Sensor by Immobilization of Natural Reagents on The Sol-Gel Monolith for pH Determination

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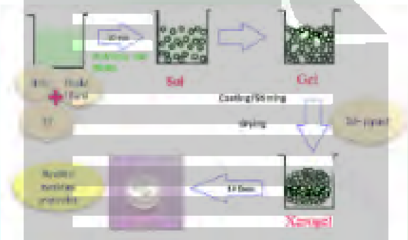
Graphical Abstract



Abstract: Due to importance of pH measurement in different aqueous environments and its effects on living creatures [1-3]. Therefore, in this study, the aim is to present a new, simple, sensitive and inexpensive analytical method based on optical sensing for pH measurement. Two optical sensors, based on the natural pigments (purple cabbage and red beetroot) doped on the sol-gel substrate, were designed and used to measure pH in different aqueous environments. The spectral properties of the prepared sensors were studied using visible spectrophotometer at their maximum absorption wavelength (530 nm for purple cabbage and 480 nm for red beetroot). The effective variables which affect on the sensor response, including of pigment concentration, temperature, speed and time of stirring in the extraction of the pigments, the amount of doped pigment and Casting and molding type of the monolith were studied and optimized. The response times of the purple cabbage and red beet pigments doped sensors are obtained less than 20 and 30 seconds and linear ranges are obtained in the pH range of 2.00 to 11.00 and 8.00 to 12.00 respectively. The relative standard deviation of both sensors with 7 repetitions is less than 1% .

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Electrosynthesis Of $ZnFe_2O_4$ Nanoparticles in An External Magnetic Field and Its Use as Adsorbent in The Removal of Dyes

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Abstract: In this study, zinc ferrite magnetic nanoparticles ($ZnFe_2O_4$) were prepared in an electrochemical cell consists of stainless steel cathode and zinc/iron anode under an external magnetic field, supplied by using two permanent NdFeB magnets arranged parallel to each other and perpendicular to the surface of electrodes. The electrolyte was a solution of CTAB 0.04 M. The current density was optimized in 18 $mA.cm^{-3}$. The nanoparticles have been characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM) and the magnetic properties were investigated by vibrating sample magnetometer (VSM). The efficiency of the prepared magnetic ZnFe2O4 nanoparticles as an adsorbent was examined for the removal of Crystal violet from water solutions, which is used in various industries including textile, plastic, and paper [1]. The presence of dyes in water creates problems for human health. Therefore removal of dyes from industrial wastewater is important for the safety of the environment [2]. The affecting parameters on the efficiency of adsorbent on the removal of Crystal violet, such as pH, amount of adsorbent, contact time, and concentration of dye were investigated. The results showed at pH 6 -7 in 90 minutes, with 3 $mg.ml^{-1}$ adsorbent, the color of the crystal violet was removed at concentrations less than 8 $mg.L^{-1}$ from water solutions. The removal mechanism is more consistent with the pseudo-second order kinetic model and by the Freundlich isotherm which shows multilayer and chemical absorption of dye on the adsorbent [3]. Based on the data of the present investigation, the biocompatible, environment-friendly, and low-cost $ZnFe_2O_4$ nanoparticles can find potential applications in wastewater treatment.

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Application of Artificial Neural Network to Modeling of Removal of TZ Dye Contaminant with HDA Modified Mt Adsorbent

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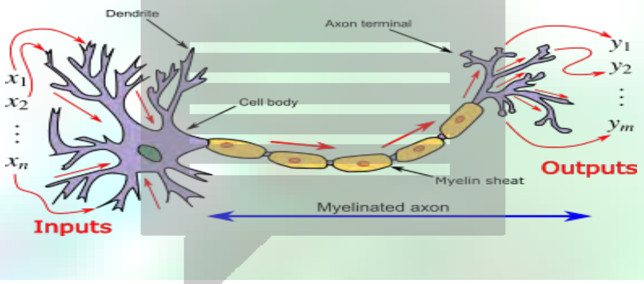
Graphical Abstract



Abstract: Artificial neural networks are a powerful and modern modeling tool, especially in cases where the relationship between data is unclear.Inspired by the way the biological nervous system works to process data and predict output responses in complex situations, and considering that the removal of color pollutants from industrial effluents is a serious environmental issue in the world, modeling these processes for Predicting the behavior of changing effective parameters can be useful .In this study, using in vitro results of tartrazine dye removal by adsorption and adsorbent of montmorillonite (MT) modified by surfactant hexadecylamine (HDA) and the effect of surfactant concentration and adsorption concentration, pH, temperature and Time, modeling and optimization with artificial neural networks .In the neural network designed using the error propagation algorithm and the reduction gradient method as a learning method and with the Adam optimizer function, the multilayer perceptron model has a data-based approach, the best Relu activator function with three hidden layers with 40,40 and 30 neurons, with 1200 epoche were determined and the best results were obtained with correlation coefficient of 0.94 and mean squares error of 0.0004. The results showed an acceptable correlation between neural network modeling and laboratory results.

Keywords: Artificial Neural Networks, Neurons, Multilayer Perceptron, Montmorillonite.

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Fabrication of Antibacterial Nanocomposite Membrane Based on PVC Polymer

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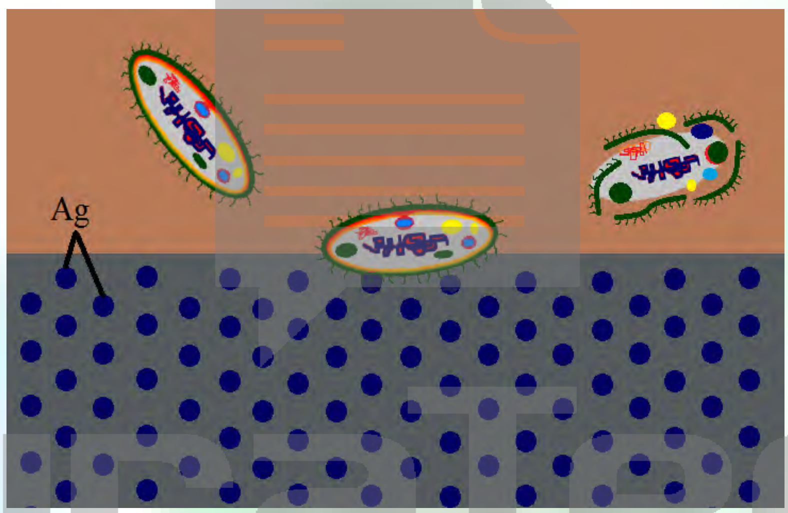
Graphical Abstract



Abstract: The significance of membrane processes for the treatment of wastewater and drinking water is still growing. The expense of membranes continues to decrease and it is possible to predict that membranes will be in extensive use in water treatment processes. Recently, the number of industrial applications has gained increasing interest. The use of antibacterial membranes in separation processes stands out owing to their considerable environmental and economic advantages. However, the evaluation of new materials for membrane fabrication opens up the opportunity for further related processes development. The composite membranes represent the essential properties of organic polymeric matrix and inorganic fillers and put forward specific advantages for the fabrication of new membranes with suitable separation performance. In this study, antibacterial nanocomposite membranes based on polyvinyl chloride polymer and silver nanoparticles were prepared using phase inversion method (immersion). For antibacterial membranes preparation, Pseudomonas bacteria were synthesized and used for antibacterial activity by weight percentage 0.25, 0.5 and 1 in the mixtures. These mixtures were then immersed in a non-solvent bath (distilled water) after being pulled by a film applicator. DLS nanoparticle analyzer was used to detect nanoparticles and particles size. Also to identify silver nanoparticles in membranes structure, X-ray diffraction (XRD) spectroscopy was used. To evaluate the antibacterial properties of the membranes Disk test was used using Escherichia coli (E. coli) as a gram-negative bacterium and Staphylococcus aureus (S. aureus) as a gram-positive bacterium. To test the performance of the fabricated membranes, the flow rate was measured and the rejection test was performed. After determining the presence of nanoparticles in the membrane structure, the DLS nanoparticle analyzer determined the size of the synthesized nanoparticles under optimal conditions between 0.46 and 0.54 nm. The permeability and antibacterial properties of membranes against gram-positive and gram-negative bacteria increased with increasing silver nanoparticles.

Keywords: Membrane, Nanocomposite, Polyvinyl Chloride, Silver Nanoparticles, Antibacterial

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Phosphorus Containing ZnO Microparticles Synthesized and Studying Physico-Chemical Features

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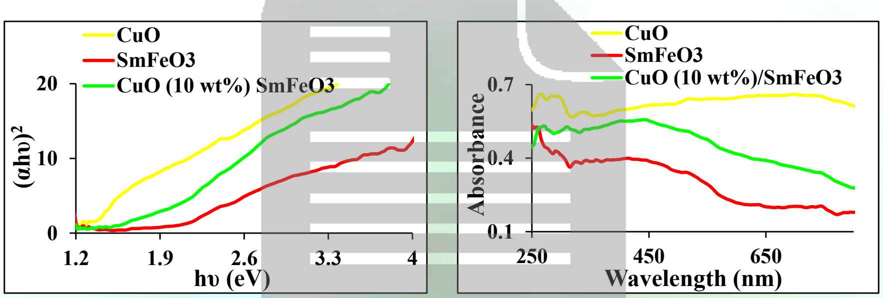
Graphical Abstract



Abstract: The semiconductor metal oxides such as TiO_2, ZnO, CuO and $SmFeO_3$ reveal appropriate photocatalytic activities due to their optical and electronic properties, low cost, chemical stability and non-toxicity [1]. $SmFeO_3$ is a rare-earth perovskite metal oxide which has been utilized in various areas [3]. CuO is one of the most important p-type semiconductors with a narrow band gap in the range of 1.2–1.9 eV which displays photoconductivity, field emission and photovoltaic properties [4]. A hybrid nanocomposite was synthesized using $SmFeO_3$ and CuO in 1:10 wt.% which was characterized by XRD, FT-IR, TEM, EDS, DRS, and UV-Vis analyses. The XRD pattern of CuO nanocrystal reveals that all of the diffraction peaks were perfectly indexed to the monoclinic CuO structure (JCPDS file no. 5-0661). Also, the XRD pattern of $SmFeO_3$ nanocrystal indicated the lattice planes of (101), (111), (200), (121), (002), (112), (220), (202), (212), (311), (123) and (242) attributed to the sharp diffraction peaks are observed at 2θ=22.82, 25.61, 31.96, 32.66, 34.04, 38.84, 39.85, 46.73, 48.39, 53.27, 59.11 and 68.50°, respectively. All of diffraction peaks were in excellent accordance with the standard XRD pattern of $SmFeO_3$ (JCPDS card No. 39-1490). The TEM images demonstrated that the $SmFeO_3$ and $SmFeO_3$/CuO(10wt%) particles were spherical like with average grain sizes of about 50 and 30 nm, respectively. The E_g values of $SmFeO_3$, CuO, and $SmFeO_3$/CuO(10wt%) were 2.01, 1.32, and 1.81 eV, respectively. The UV-Vis absorption spectra exhibited that the CuO nanoparticles absorbed visible light in the range of 400–800 nm due to their narrow band gap (E_g=1.32 eV) while $SmFeO_3$ nanoparticles absorbed lower amount of light in the range of 300-600 nm (E_g=2.01 eV). The $SmFeO_3$/CuO(10wt%) composite demonstrated the highest visible light absorption in the

spectral range of 300-600 nm. Thus, it was anticipated that this material will exhibit the most remarkable photocatalytic activity.

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Photocatalytic Degradation of Organic Pollutants Using $SmFeO_3/CuO$ Nanocomposite Photocatalyst

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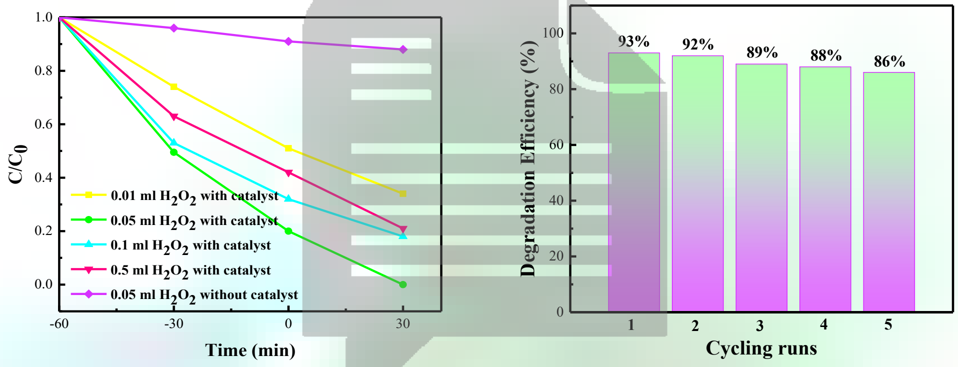
Graphical Abstract



Abstract: Many hazardous chemical compounds including dyes and other toxic organic materials formed from a textile and clothing industry wastewater would bring about severe pollution in the Earth's environment [1,2]. Several methods have so far been used for water treatment including adsorption and advanced oxidation processes (AOPs) [3,4]. In this work, hybrid nanocomposite $SmFeO_3/CuO$(10wt%) photocatalyst was synthesized, characterized and its capability for RhB dye and phenol degradation was explored under the visible light irradiation. The highest photocatalytic efficiency of 65% was achieved under the visible light irradiation for the degradation of 8 mg/L RhB dye using 0.15 g $SmFeO_3/CuO$(10wt%) catalyst at pH=5. The photocatalytic activity was reached to 100% using 0.05mL of H_2O_2 under the above-mentioned optimized conditions. Moreover, the optimum $SmFeO_3/CuO$(10wt%) catalyst illustrated 93 and 85% performances for the degradation of 20 mg/L RhB dye and phenol in presence of 0.05 mL H_2O_2 confirming the occurrence of both Fenton-like oxidation and photocatalytic mechanisms. The trapping experiments proved that the hydroxide radicals had a key role in degradation of RhB over the $SmFeO_3/CuO$(10wt%) nanocomposite photocatalyst. Finally, it could be suggested that the $SmFeO_3/CuO$(10wt%) hybrid photocatalyst can find potential applications in industrial water treatment processes due to it is a highly stable and active sample.

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Theoretical Investigation of Carbonic Anhydrase Enzyme Catalytic Cycle as Biocatalyst in Carbon Dioxide Hydration

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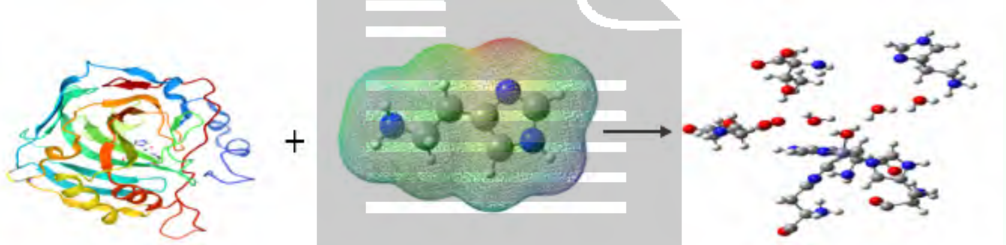
Graphical Abstract



Abstract: The hydration of carbon dioxide (CO_2) to bicarbonate ion and proton, a simple but essential reaction, is catalyzed by a family of ubiquitous zinc metalloenzymes known as carbonic anhydrase (CAs, EC 4.2.1.1) [1, 2]. This enzyme (CA) present in prokaryotes and eukaryotes and encoded to five classes: α-CAs, β-CAs, γ-CAs, δ-CAs and ζ-CAs [3]. In the present research we explored the interaction between some of new activators and histamine as reference activator with human carbonic anhydrase cluster model, using quantum mechanical calculations, based on the DFT, quantum theory of atoms in molecules (QTAIM) and natural bond orbital (NBO). The obtained results indicate that the activator molecule participates in proton transfer reactions by forming CA-activator complexes and enhances the formation of the active species of CA, the zinc hydroxide species. Moreover, bridging the two water molecules between activators molecules and CA active site, results in the formation of thermodynamically more stable CA-activator complexes. The results of our modeling could be useful in examining the long-range proton transfer processes and evaluating the role of hydrogen-bounded water networks. As CA activators recently emerged as interesting agents for enhancing cognition, in the management of carbonic anhydrasr

deficiencies, or for therapy memory, these potent hCA activators may be considered of interest for in vivo investigations and for possible therapeutic applications. The good agreement between these theoretical results and the experimental data confirm the accuracy level of our calculations, able to predict the interaction site of newly designed CAAs, at least with the model active site of the enzyme.

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Determination of Ni^{2+} in Aqueous Solution by Ion Selective Electrode at Screen Printed Electrode Modified by Ion Imprinted Polymer

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Abstract: For many decades, nickel was regarded as a potentially toxic element, since its concentration in various foods was higher than that needed for living organisms. More recently, it is now considered a possible essential element for plants, although deficiencies can occur under certain circumstances. However, nickel can be toxic at high concentrations and can be a problem in some soils. Hence the need for nickel ion determination in clinical and food analysis and environmental monitoring has led to a number of methods for the measurement of this analyte [1].The Nickle ion-imprinted polymer particles(IIP) were synthesized via single pot method by dissolving of ternary complex of Nickle with 5, 7-Dichloroquinoline-8-ol (DCQ) and 4-vinyl pyridine (VP) in acetonitrile (porogen) and copolymerized thermally after addition of methyl methacrylate (monomer) and ethylene glycoldimethacrylate (crosslinking monomer) in the presence of 2,2-azobisisobutyronitrile (initiator). The bare screen printed electrode were prepared and constructed according to the procedure described elsewhere [2].The chemically modified screen printed electrode electrodes were prepared by thoroughly mixing of PVC, NPOE, NaTPB and nickle IIP particles (60–85µm size) in proportions of 27, 53, 5 and 15% (w/w), respectively and dispersed in 2.5 ml of tetrahydrofuran (THF). The mixture was homogenized in a sonicator and then poured into a watch glass. The THF solvent was allowed to evaporate at room temperature to obtain a viscose mixture, to cover the screen printed electrode surface. The solvent was allowed to evaporate to thin PVC film formed on the screen printed electrode surface. The plot obtained for the sensor with Nickle IIP particles showed a slope of 29.2 mV per decade over a concentration range of 5.0×10^{-6} to 1.0×10^{-4}M of Nickle is the expected Nernstian slope for the divalent cations. The limit of detection was 1×10^{-7}M Nickle calculated based on the IUPAC definition. However, the electrode with the blank membrane showed no response for Ni ion in the concentration range 5.0×10^{-6} to 1.0×10^{-4}M. The electrode was used in the direct determination of Ni^{2+} in aqueous solution. Selectivity parameter data for various ions are presented in table .1.

Table.1.Potentiometric selectivity coefficient values, $K^{pot}_{Ni,M}$

M^{n+}	Na^+	K^+	Ca^{2+}	Mg^{2+}	Cu^{2+}	Zn^{2+}
$K^{pot}_{Ni,M}$	5×10^{-4}	6×10^{-4}	1×10^{-3}	4×10^{-4}	1×10^{-3}	2×10^{-3}

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The Preparation Method and Properies of One-Component Epoxy Powder Adhesive as Green Adhesive

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Graphical Abstract

Abstract: Today, adhesive joints are considered as one of the most widely used bonding methods in various industries due to their high strength-to-weight ratio, uniform stress distribution, and desirable appearance. The reduction volatile organic compound (VOC) emissions is one of the most important issues in the preparation of green adhesives. Epoxy adhesives are one of the most common reactive adhesives used in solid, liquid and paste forms due to their high mechanical and chemical resistance. These types of adhesives are used as one-component and two-component. In this paper, one-component epoxy powder adhesives prepared by solvent evaporation are investigated. Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and differential scanning calorimetry (DSC) were used for characterization of this type of adhesives. Adhesive properties of this green adhesive has been evaluated in terms of the lap shear

strength using aluminium adherends. The results showed that in one-component powder adhesive (green adhesive), however the epoxy chains were in contact with imidazole curing agent for long time (seven years), it was still thermoplastic. Anionic polymerization of epoxy in presence of imidazole increased the chain length of solid epoxy in one-component powder adhesive so that its melting temperature is increased. On the other hand, all the epoxy functional groups of one-component powder adhesive do not participate in the curing reaction with imidazole curing agent. This green adhesive durability in various curing temperature has also been analysed. The results indicate that this one-component epoxy powder adhesive presents a higher adhesive strength at curing temperature of 150 °C.

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Biocompatible Adsorbent for Drug Storage and Removal Applications: A Molecular Dynamics Study

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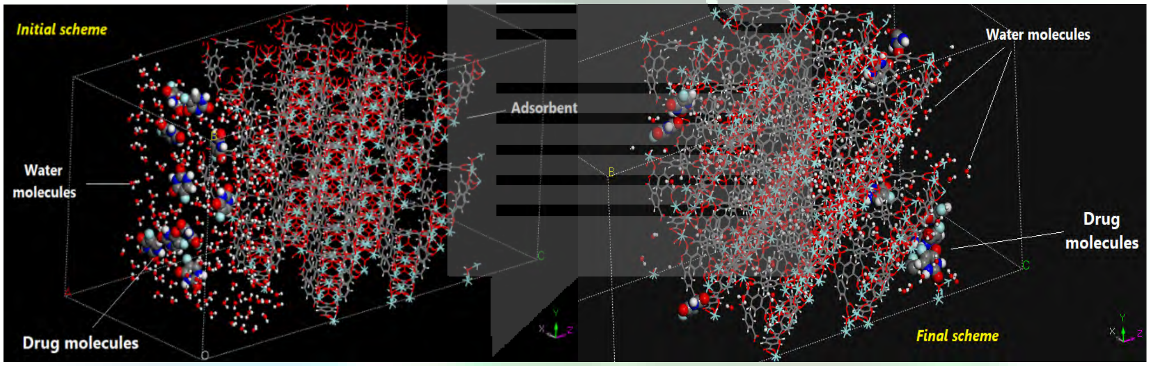
Graphical Abstract



Abstract: Water pollutants can be classified as many kinds such as organics and inorganics that mainly are discharged from industrial effluents and human sewage into the water [1]. Metal Organic Frameworks (MOFs) have been used widely as molecular adsorbent due to their large surface area, high pore volume, high payload, low toxicity and biocompatibility [2-3]. MOF drug delivery system (DDS) can prevent drug release into the water by restricting the drugs into MOFs. In addition, DDS can also reduce the side effects of anticancer drugs while they circulate into the body [4]; MOFs can be used as filters [5]. In this study, we investigated two anticancer drugs, 5-fluorouracil (5-FU) and gemcitabine (GEM), diffusion and storage into UiO-66 by molecular dynamic (MD) simulations. In order to gauge diffusion of 5-FU and GEM into UiO-66, mean square displacement (MSD) was computed for both promising drugs. MD simulations show an acceptable adsorption and diffusion of 5-Fu in MOF unlike GEM drug. Adsorption of GEM was

mostly on exterior sites of UiO-66 due to high diameter of GEM than the diameter of UiO-66 pores.

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Quntum Mechanical Study on Interaction Between Carbonic Anhydrase Bio Catalyst Model Enzyme with New Class of Inhibitors

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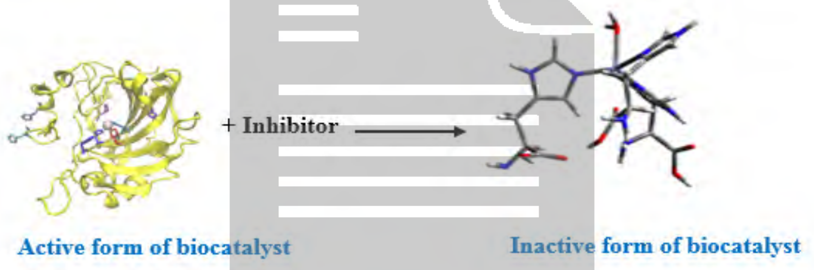
Graphical Abstract



Abstract: Carbonic anhydrases (CAs) are a superfamily of metallo-enzymes, which catalyzed the reversible and simple reaction of carbon dioxide hydration to bicarbonate and proton, eq 1.

$$CO_2 + H_2O \longrightarrow HCO_3^- + H^+ \qquad (1)$$

There are five genetically distinct groups of carbonic anhydrase enzymes known as α, β, γ, δ and ζ [1-3]. α-CA as the first and the most important group of the carbonic anhydrase family, has been found in vertebrates, monocytes, algae, and finally in the cytoplasm of green plants and in some bacteria. In the present research a new class inhibitors of different carbonic anhydrase (CA) isoforms are investigated using DFT calculations. The most advantage of DFT method is a significant increase in computational accuracy without the additional increase in computing time. The harmonic vibrational frequencies were calculated to confirm that a full optimized structure correctly corresponds to a local minimum which has only real frequencies. In addition, the vibrational frequencies have been employed to obtain enthalpies and Gibbs free energies at 298.15

K and 1.0 atmosphere pressure. All calculated enthalpies were zero-point (ZPE) corrected with unscaled frequencies. Our results indicate that these kind of inhibitors, inhibited the human carbonic anhydrase with very different inhibition profiles compared to other inhibitors. According to calculated results, studied inhibitors are anchored to the non-protein zinc ligand (hydroxyl ion) by means of a hydrogen bond and an intermediate complex is formed, $[(his)_3Zn(II)(OH)/inhibitor]$, which is in good agreement with experimental data. In continue the active form of the CA enzyme converted to inactive form. Finally, the HOMO-LUMO and AIM analysis have been done to understand the details of interaction between studied inhibitors and CA active center in intermediate complex in solvent phase.

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Fabrication of Nanofiltration Membrane Based on A Mixture of Poly(vinyl Chloride) and Poly(Methyl Methacrylate) Polymers for Separation of Bivalent Water Ions

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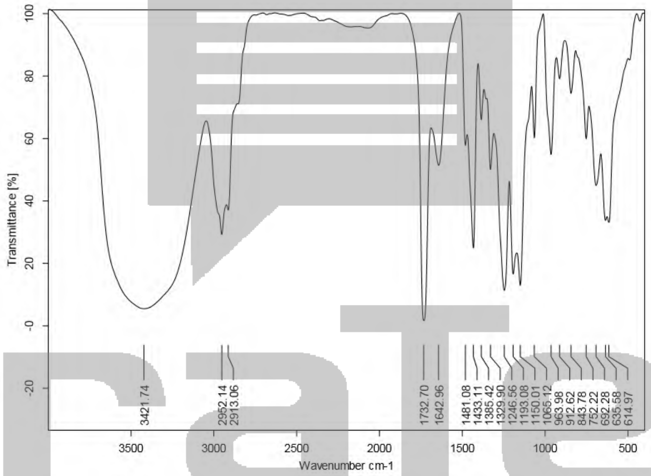
Graphical Abstract



Abstract: The global problem of the scarcity of drinking water resources, caused by various reasons such as pollution from human activities, environmental degradation and climate change, has affected human life all over the world. One of the best and most effective ways available to solve this challenge is wastewater treatment. Membrane processes for water treatment plants are new methods that have been developed over the last fifty years. These new processes have many advantages, such as low current cost and high efficiency. In a membrane process, there are generally two phases that are physically separated by a third phase (membrane). The membrane controls the mass transfer between the two phases. Membranes, which are considered as the heart

of the membrane process, are prepared with different structures. Nanofiltration is one of the most widely used membrane processes that has been used in various industrial and commercial fields and new applications have been planned for it. One of the applications considered for membrane processes is the separation of different water ions. For example, the purification of drinking and agricultural water from heavy binary metals, which often cause many environmental problems due to their toxicity, can be carried out by membrane processes. In this study, using the phase inversion method, a nanofiltration membrane was fabricated on the basis of a mixture of poly(vinyl chloride) and poly(methyl methacrylate) polymers. For this work, tetrahydrofuran was used as a solvent. Experimental design method using Taguchi model was used to obtain the optimal membrane and also FT-IR spectroscopy was used to investigate the formation of the desired chemical bonds .In the experimental design, three factors including weight percentage of polymers, solvent evaporation time and membrane thickness were considered as variables and two factors including flow rate and rejection were considered as dependent variables or response variables. It was found that the best miscibility ratio of polymers is 70% poly(vinyl chloride) to 30% poly(methyl methacrylate) .Also, the desired membrane was obtained at a concentration of 14% by weight of polymers, solvent evaporation time of 15 seconds and membrane thickness of 150 µm.

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Removal of Organic Dye by Yb-doped PbTe Nanomaterial: Synthesis, Characterization and Photocatalytic Investigation

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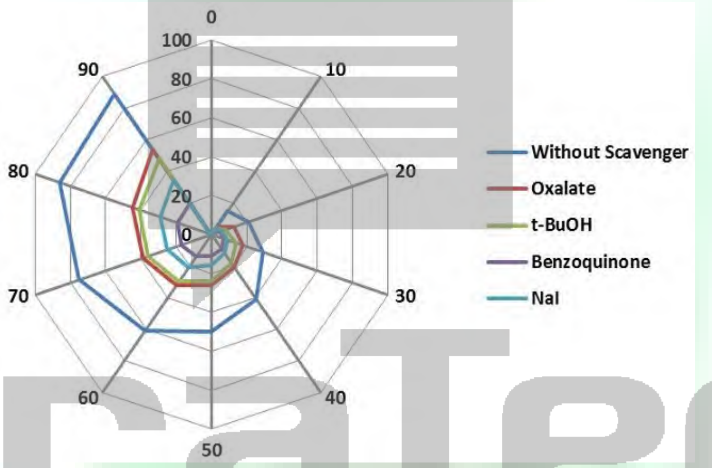
Graphical Abstract



Abstract: Nowadays, water contamination and world energy crisis have attracted much amused attention among scientific communities. Recently, modified Ln^{3+}-doped semiconductors have been used as effective catalyst by controlling the recombination probability of produced electron-hole pairs in semiconductors In this study, Yb-doped PbTe nanoparticles with variable Yb^{3+} content were synthesized by a simple hydrothermal technique. The synthesized nanoparticles were characterized by X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and powder X-ray diffraction (XRD). The XRD patterns indicated that the particles were excellently crystallized due to the cubic PbTe phase. The SEM images certify that the substitution of Yb into the lattice of PbTe does not change the morphology of PbTe nanoparticles. The SEM images displayed that the size of the particles was in the range of 20-70 nm. The energy of the

bandgap of doped-PbTe and PbTe nanoparticles expected from the chief absorption edges of the UV-Vis diffuse reflectance spectrum. Blue shifts in DRS spectra of PbTe were noticed by increasing the concentration of the Yb^{3+} ions. The incorporation of Yb^{3+} into the PbTe lattice was confirmed by the XPS technique. The electrical conductance of various Tb-doped PbTe samples is higher than that for the pure PbTe, and elevates with temperature. The photocatalytic performance of Yb-doped PbTe compounds was determined as well by Malachite green (MG) degradation under visible light irradiation. Improved photocatalytic activity was shown for Yb-doped CdTe with 0.1mol Yb dopant. Considering radical scavengers, the sequence of inhibitory effect was 1, 4 Benzoquinone > I^- > t-BuOH > $C_2O_4^{2-}$**.** The influence of various specifications like catalyst amount, primary dye concentration, and ultrasonic power were explored. The enhanced photocatalytic performance can be attributed to the electron transfer between Yb^{3+} and PbTe by introduction of an Yb 4f level.

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Investigating Outstanding Properties of Phosphorus Containing ZnO Microparticles Synthesized Through Hydrothermal Process

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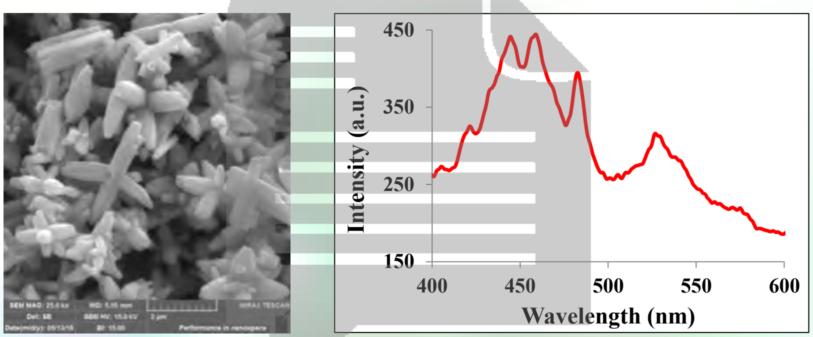
Graphical Abstract



Abstract: Zinc oxide is attracted great attention as it indicates a high photocatalytic efficiency similar to or greater than titanium dioxide, good biocompatibility and environmental stability [1]. ZnO can replace TiO_2 because of its physical and chemical properties and also its bandgap which is similar to that of the TiO_2. The ultraviolet wavelengths should be used due to the large bandgap of the ZnO [2]. However, the charge carriers' recombination in ZnO is relatively high which restricts its extensive application in the photocatalytic reactions. To tackle this challenge, diverse methods have been adopted. Non-metal and metal doping is an effective method for reducing band gap and improving charge carriers' separation and changing the wavelength threshold of absobed light to the visible area [3]. In this research, a phosphorus containing ZnO photocatalyst containing 1.8 wt.% of phosphorus (ZnO-P1.8%) was successfully synthesized using the hydrothermal method. The structural, physical and optical properties of the obtained microparticles were investigated using varied methods including scanning electron microscopy (SEM) image, X-ray diffraction (XRD), Fourier transform infrared (FT-IR) spectroscopy, ultraviolet-visible diffusion reflectance spectroscopy (UV-Vis DRS), and photoluminescence (PL) spectroscopy. The SEM image illustrated that the ZnO-P1.8% had a rod-like morphology so that some rods were joint together to form a flower-like shape but some of the rods were isolated and exhibited regular hexagonal and/or conical shapes. The PL spectrum showed six peaks in the range of 400 to 600 nm including a broad peak near 420 nm, three sharp peaks at around 445, 460 and 480 nm along with two broad peaks at about 530 and 575 nm.

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Application of Phosphorus Containing ZnO Microparticles in Water Treatment Through Photocatalytic Degradation of Contaminants Under Visible Light Radiation

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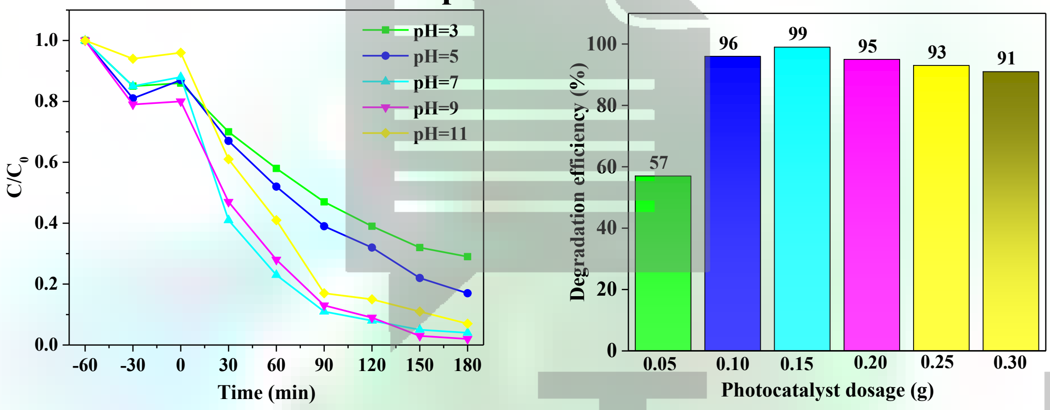
Graphical Abstract



Abstract: The water treatment is one of the most critical issues worldwide because of the population growth and environmental problems [1]. There are advanced technologies used for the water treatment. One of these technologies is the photocatalytic degradation of organic pollutants using photocatalysts such as ZnO that nowadays are widely used because of their visible light absorbance ability and low costs [2,3]. Photocatalysts are semiconductor solid oxides which can create electron-hole pairs upon light absorption. These electron-hole pairs react with existing materials at the surface and oxidize them to low-risk materials [4]. The photocatalytic activity of the photocatalyst containing 1.8 wt.% of phosphorus, i.e. P-ZnO1.8% sample, was evaluated for the degradation of Rhodamine B (RhB) under visible light irradiation. The parameters such as pH, catalyst dosage, contaminant concentration and effect of persulfate as an oxidant were studied. It was found that the P-ZnO1.8% photocatalyst could destroy 99% of RhB (5 ppm) in 180 min at pH=7; furthermore, it degraded ~100% of 5 and 10 ppm of the RhB pollutant in 120 and 180 min, respectively, only by adding 0.01 g of persulfate into the reaction solution. According to the reusability test, it was proved that after five cycles, the catalyst activity was not highly changed and it was potentially capable of pollutant degradation.

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Impact of Using Fin in Phase Change Material for Energy Storage System

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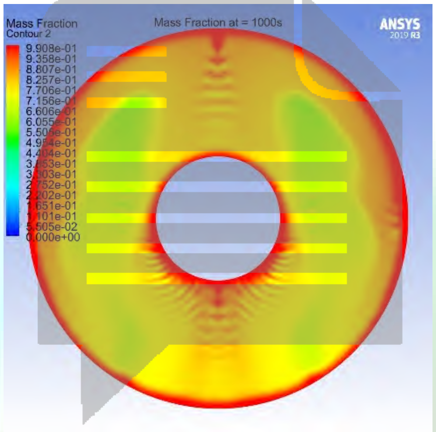
Graphical Abstract



Abstract: In this work, an analysis of Pipes with and without fins with phase change material (PCM) based energy storage system. This analysis is simulated with the help of ANSYS Fluent V19. PCMs have many applications in thermal energy storage due to their high ability to latent heat storage. due to this feature, the use of PCMs in the storage of thermal energy from solar sources is widely used. In this work, an attempt has been made to investigate the impact of using fins in the design of structures used in energy storage with the help of PCMs. In two separate designs, PCM materials were placed in equal volumes in the structure. In the first design, the material was without a fin and in the second design, with the help of 4 fins, it was placed in the designed structure with a 90 degree angle. The results showed that the use of fins increased the melting rate of the material. The results also showed that the presence of fins can increase the heat transfer rate in PCM materials.

Keywords: PCM, Ansys Fluent, energy storage

Synthesis, Characteristics and Photocatalytic Degradation of The Metronidazole from Aqueous Solution by ZnO Nanoparticles Immobilized on A Stone Surface

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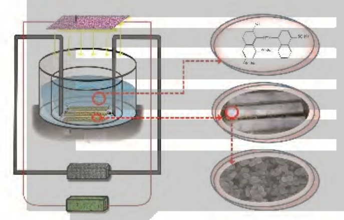
Graphical Abstract



Abstract: The presence of antibiotics such as metronidazole in wastewater even at low concentrations requires searching for a suitable process such as advanced oxidation process (AOP) to reduce the level of pollutants to a standard level in water. In this study, zinc oxide (ZnO) nanoparticles were synthesized by thermal method using zinc sulfate (ZnSO4) as a precursor, then, stabilized on stone and was used as a catalyst, in order to degrade metronidazole by photocalytic process. Effective factors on the removal efficiency of metronidazole including the initial metronidazole concentration, contact time, pH, and 0.9 gL^{-1} ZnO stabilized on the stone surface were investigated.The X-ray diffraction (XRD) studies showed that the synthesized nanomaterials have hexagonal Wurtzite structure. Also, scanning electron microscopy (SEM) analysis revealed that the average crystalline size of the synthesized ZnO particles was in the range of 1.9-3.2 nm. The spectra represented a sharp absorption edge at 390 nm for ZnO nanoparticles corresponding to band gap of 3.168 eV. The maximum removal efficiency was 98.36% for the synthetic solution under a specific condition (pH = 11, reaction time = 90 minutes, ZnO concentration = 0.9 gL^{-1}, and the initial concentration of metronidazole = 10 mgL^{-1}). The photocatalytic degradation was found to follow pseudo-first-order degradation kinetics. Therefore, the ZnO nanoparticles synthesized by thermal decomposition are suitable and effective photocatalytic materials for degradation of pharmaceutical contaminants.

Keywords: ZnO, Metronidazole, UV, Nanoparticles, Degrediation

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On-chip Electromembrane Extraction with Monolithic Adsorbent in Acceptor Phase

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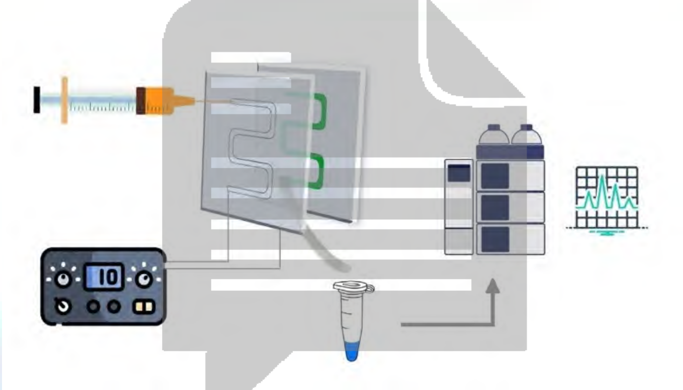
Graphical Abstract



Abstract: Non-steroidal anti-inflammatory drugs (NSAIDs) are one the most commonly prescribed pain killers. NSAIDs can cause adverse health effects on humans such as gastrointestinal disorder, anemia, agranulocytosis and changes in renal functions. Therefore, it is significant to achieve a suitable technique for accurate measuring these compounds. During the last decades, many studies have focused on development of simple, environmentally friendly and efficient miniaturized sample preparation methods with a high clean up ability. In this way, a lot of extraction techniques such as solid phase microextraction (SPME) and electromembrane extraction (EME) have been employed in remarkable number of investigations. As a result of performing two extraction techniques simultaneously, it could be possible to take advantages of both methods. Hence, extraction recoveries, preconcentration factors and other noteworthy extraction features such as ability to clean up through matrix sample could be improved. In this study, Cu/Cr layered double hydroxid was dispersed in poly (methacrilic acid-coethylene glycol dimethacrylate) (MAA-co-EGDMA) polymerization mixture and in-situ polymerization was performed in acceptor phase

channel. Thus, a monolithic composite was formed in the channel. Thereafter, EME-SPME on chip was developed to extract naproxen, diclofenac and mefenamic acid from various complex matrices. Likewise, desorbtion step was performed after electromembrane extraction and eluent was injected into high performance liquid chromatography-UV for separation and determination of the drugs. Effective parameters on extraction efficiency were optimized and under optimum conditions, the limit of detections of the mentioned analytes were 0.1-0.25 ng/mL. Linearity of method was obtained within the range of 0.5-500 ng/mL for naproxen and 1-250 ng/mL for dicofenac and mefenamic acid with coefficients of determination greater than 0.996. Under evaluation of this method, extraction recoveries were obtained in the range of 83.34-90.87% which corresponded to preconcentration factors of 56-61. The precision of the method is suitable with relative standard deviations lower than 4.8%. The method was applied for extraction of the drugs from real saples like as breast milk, urine and plasma; and satisfactory results were obtained.

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Variations in *Zataria multiflora* Essential Oil Content in Response to Green Synthesized Zinc-Oxide Nanoparticles

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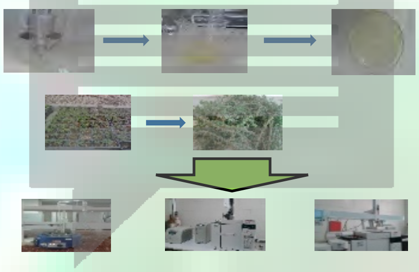

Abstract: Since the desires for nanoparticle (NP) applications in agriculture increase, their green and sustainable synthesis has attracted more attention. Large scale applications of chemical fertilizers not only disturb the soil mineral balance but also reduce soil fertility. NPs can enhance crop productivity by increasing the photosynthetic activity, the rate of seed germination, seedling growth, metabolism of the nitrogen, carbohydrate and protein synthesis. Zinc oxide nanoparticles (ZnO NPs) are among the most commonly used NPs in agriculture [1]. Chemical components and the yield of essential oils (EOs) correlate with the amounts of nutrients that are available to plants [2]. The present study was planned to determine the variations in *Zataria multiflora* Boiss EO content in response to green synthesized ZnO NPs. ZnO NPs were synthesized via ultrasonic irradiations by using the extracts of *Punica granatum* and *Citrus aurantifolia* pomaces to evaluate their foliar application in different concentrations (0, 100 and 300 mgL^{-1}) on EO yield and composition of *Z. multiflora* in comparison to the Zn-EDTA fertilizer, separately. The Pomaces were gathered from a juice factory in Jahrom, Fars province (south of Iran). The extracts from each pomaces were prepared based on previous report [3,4]. The seedlings of *Z. multiflora* were produced under greenhouse controlled environment. The seedlings were planted based on a randomized complete block design. The plants were irrigated at interval of 4 days. 20 days after transplanting, ZnO NPs with different concentrations (0 - distilled water, 100 and 300 mgL^{-1}) were sprayed on the plants every 10 days. At the end of the plant growth period, the plants were dried at laboratory condition. After that, the EO was extracted from aerial part of plant using a Clevenger-type apparatus. Analyses of the volatile oils were carried out by gas chromatography (GC-FID) and by gas chromatography-mass spectrometry (GC-MS). The biggest amount of EOs yields were found in ZnO NPs synthesized by *Punica* pomace and at 300 mgL^{-1} concentration. Zn-EDTA fertilizer at 100 mgL^{-1} concentration was shown the high yield of EO in ZnO NPs synthesized by *Citrus* pomace. The predominant component in *Z. multiflora* EO was linalool in all of the plants that had received treatments. According to the obtained results, the plant responses to the evaluated ZnO NPs were not the same. Different sources of zinc fertilizer significantly enhanced oxygenated monoterpenes content.

Keywords: Nanoparticles, Essential oil, Pomaces, *Zataria multiflora*, Zinc fertilizer.

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Capacitive Sensor Based on Green Synthesized Graphene Aerogel Nanocomposite

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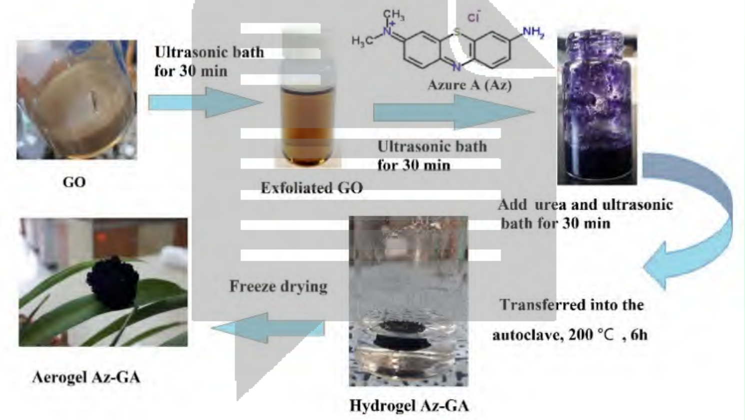
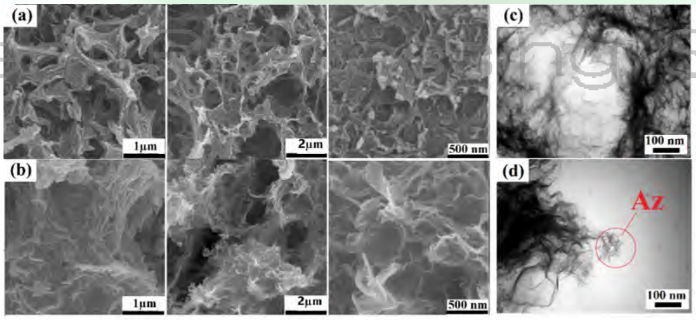
Graphical Abstract

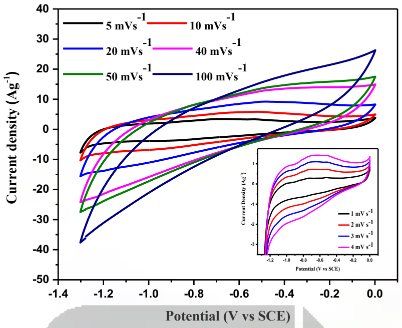


Abstract: The use of renewable energy, such as solar and wind power, is of great importance to meet the energy demands of a growing population, as non-renewable energy sources dwindle and the general public gain more knowledge on environmental pollution. One of the most important challenges in the energy storage industry is the design of energy storage devices from sustainable sources that have high energy capacity and high power capability[1-3]. 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[4,5]. To this aim, herein, azure A/3D graphene aerogel (Az–GA) redox-active electrodes are fabricated via a hydrothermal and green method. Az links to 3D GA via π–π interactions to form an anode. The new electrodes were synthesized via a one-step hydrothermal process and electrochemically characterized via cyclic

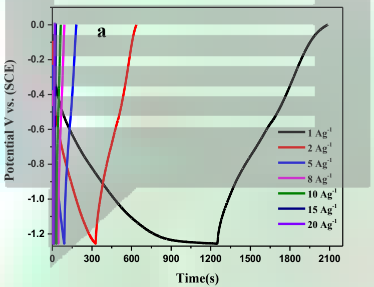
voltammetry (CV) and galvanostatic charge-discharge (GCD) measurements. A modified Hummers' method was used to synthesize graphene oxide (GO). To prepare Az–GA via a hydrothermal method, GO (25 mg) was dispersed in water (10 mL) in an ultrasonic bath for 30 min. Then, a specific amount of Az chloride was added into the dispersed GO mixture, which was then ultrasonicated for a further 30 min, during which time the color of the mixture changed from light brown to dark blue. Then, urea (500 mg) as a reducing agent was added to the mixture, which was ultrasonicated for around a further 10 min. Next, the mixture was transferred into a 50 mL Teflon-lined stainless steel autoclave and heated at 200 °C for 6 h. The Az–GA was suspended on top of the solution, indicating the complete adsorption of azure molecules into the GA structure. The synthesized Az–GA was washed with a large amount of DI water to remove the impurities from the product. Finally, the Az–GA was frozen at −70 °C and dried under vacuum. The same method was used to prepare Pure GA. An Az–GA/NF electrode was made using nickel foam as a current collector with a surface area of 1.0 cm2 and 3 M of KOH as an aqueous electrolyte. The nickel foam was then coated with a slurry containing 85 wt.% of Az–GA, 10 wt.% of carbon black, 5 wt.% of PVDF, N-methyl-2-pyrrolidone (NMP), and a small amount of DI water and pressed under 5 MPs for 10 s and dried at 60 °C for 12 h. Around 1 mg of Az–GA was deposited on the NF as an anode for a supercapacitor. The Az–GA electrode exhibits good electrochemical performance and high specific capacitance of 716.06 F g−1 at a current density of 1 A g−1.



FE-SEM and TEM images of (a and c) GA and (b and d) Az–GA.



CVs of the Az–GA/NF electrode at various scan rates from 5 to 100 mV s^{-1}, (inset: CVs of scan rates from 1 to 4 mV s^{-1}) 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^{-1} in aqueous 3 M KOH electrolyte

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Electrochemical Impedance Spectroscopy Study of The Response of Phthalic Acid Esters on The Azolla Modified Copper Electrode

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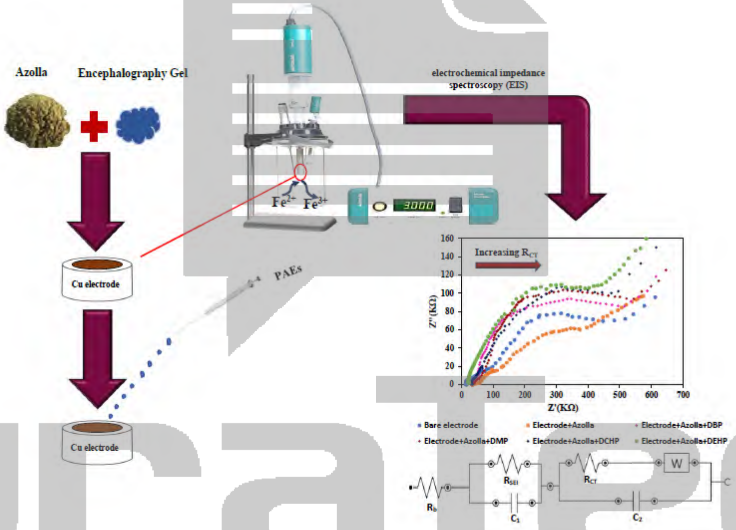
Graphical Abstract



Abstract: Phthalic acid esters (PAEs) are a group of hand-made chemicals used as softener, stabilizer or additive in many consumers and industrial products. Humans are exposed to these substances throughout their lives, even in the womb through maternal contact [1]. They lower testosterone and cause abnormalities in the male reproductive system and may cause carcinogenic effects and genetic damage. These substances may enter the environment during production, use or destruction of products and cause pollution to water, soil and atmosphere [2]. In this work, a sensitive and efficient electrochemical sensor was introduced and the interacton of four phthalic acid esters (PAEs) including dibutyl phthalate (DBP), dimethyl phthalate (DMP*), di(2-ethylhexyl) phthalate* (DEHP) and dicyclohexyl phthalate (DCHP) in aqueous solutions with this biosensor was separately investigated by electrochemical impedance spectroscopy (EIS). The

surface of a copper electrode was modified by azolla paste prepared using azolla powder and the electroencephalography gel (EEG). For this purpose, sufficient amount of azolla fern was collected from Anzali wetland, washed by deionized water, dryied and grounded to produce powders with the particle size of < 74 microns. The azolla powder was characterized by FESEM, TEM, BET, FT-IR and EDX methods. Determination of PAEs was conducted based on their blocking effect on the electrode surface for ferrous ions oxidation. Due to the Nyquist plots, the charge transfer resistance (R_{CT}) of bare electrode and azolla modified electrode were 468.8 and 438.7 kΩ, respectively. After separately injection of 3 μg L^{-1} DBP, DMP, DEHP and DCHP, R_{CT} were obtained as 563.9, 588.5, 548.7 and 570.1 kΩ, respectively. By taking a closer look, spatial hindrance of PAEs play major role in R_{CT} shifts. The blockers with smaller structure provide the better point-by-point coverage of surface which conclude the bigger shift in the R_{CT}. So, the blocking properties of PAEs was confirmed. The above-mentioned results, give us exciting sign of future opportunity for developing the impedimetric biosensor of PAEs. This biosensor will work based on the R_{CT} shifts versus PAEs concentration. It is clear that the small changes in carbonyl group polarity in the PAEs structure will affect ΔR_{CT} and bring selectivity for impedimetric biosensor of PAEs. According to the results this biosensor can be used to determine PAEs in real aqueous samples.

Keywords: Azolla modified electrode, Biosensor, Phthalic acid esters, Electrochemical impedance spectroscopy.

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Mechanical, Chemical, Physical and Antimicrobial Properties of Chitosan-Based Film Incorporated with Walnut Septum

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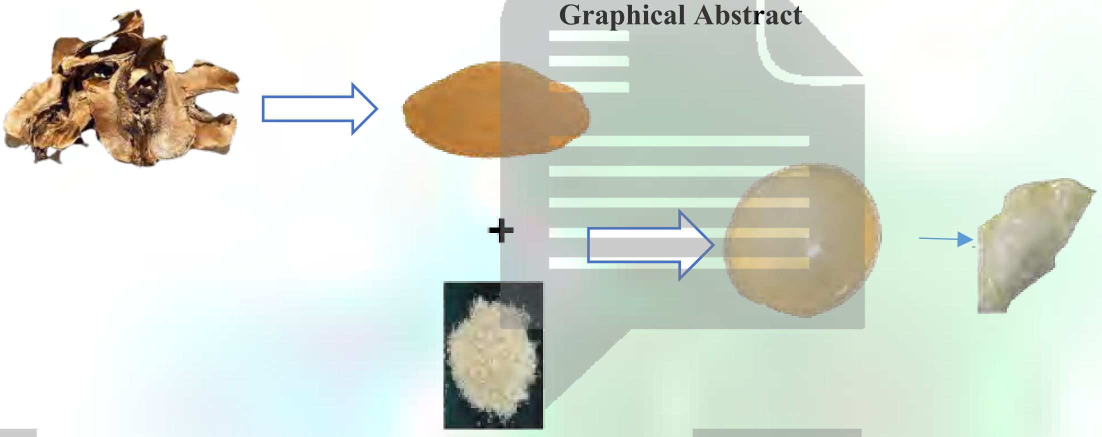
Graphical Abstract



Abstract: Chitosan films incorporated with various concentrations of raw walnut septum powder were prepared and investigated for the production of biodegradable plastics, especially in packaging to improve the quality, delay the spoilage of packaged food, as well as increase the safety and shelf life of food. Walnut septum ultrafine powder was produced with the following steps selecting raw materials, cleaning, drying, freezing, and rapidly placing the frozen walnut septum in a crusher and then crushing and screening the walnut septum powder. So as to obtained the walnut septum (WNS) ultrafine powder having crushing granularity being 300 meshes.

In the present study, the efficacy of response surface models was analysed to optimize experimental conditions for maximum improve of film thickness (FT), Tensile strength (TS), elongation at break (EB) water vapor permeability (WVP) and oxygen permeability (OP).

The estimated overall optimum conditions by overlaying the responses of BoxBehnken design of response surface methodology were found to be FT=0.097±0.005 (chitosan without WNS= 0.101±0.06) TS=29.581±0.381 (13.871±0.631), EB=34.12±2.15 (31.97±1.33), WVP=2.11±0.05 (2.66±0.03)$\times 10^{-10}$ and OP=0.48±0.05 (1.41±0.04)$\times 10^{-18}$

In optimum condition, chitosan films incorporated with WNS showed the strongest antimicrobial activity and was significantly increased in tensile strength (TS) of film and decreased water vapor permeability and oxygen permeability. Microstructure of the film incorporated with WNS was investigated by Fourier transform infrared spectroscopy and scanning electron microscopy (SEM) and it was Found WNS was dispersed homogenously into chitosan matrix. Surface morphology of the film with WNS revealed a homogeneous structure. Overall, chitosan films with WNS could be used as novel food packaging material due to their excellent antimicrobial and mechanical properties.

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Performance of A Chemical Colorimetric Sensor to Determine Silver Ions and Ephedrine

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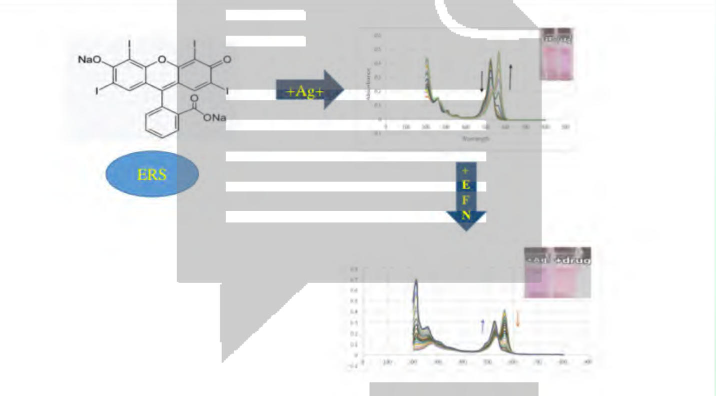
Graphical Abstract



Abstract: In this study, the efficacy of erythrosine for the determination of silver ions and the drug ephedrine was investigated. Erythrosine acts as a colorimetric sensor in a simple and selective way to detect silver ions by changing color and changing the absorption spectrum. The resulting complex can act selectively as a receptor for the identification of ephedrine in aqueous media. The linear ranges for silver cation and ephedrine are 0.094-0.147 and 11.52-192.45 microloles per liter, respectively, and their correlation coefficients are 0.9897 and 0.9941, respectively. In addition, their detection limits were calculated as 0.0001 and 4.06 micromoles per liter

Keywords: Chemical sensors, erythrosine, silver cation, ephedrine

Green Synthesis of Nitrogen and Sulfur-Doped Carbon Dots for Fluorometric Determination of Pd^{2+} and Fe^{3+}

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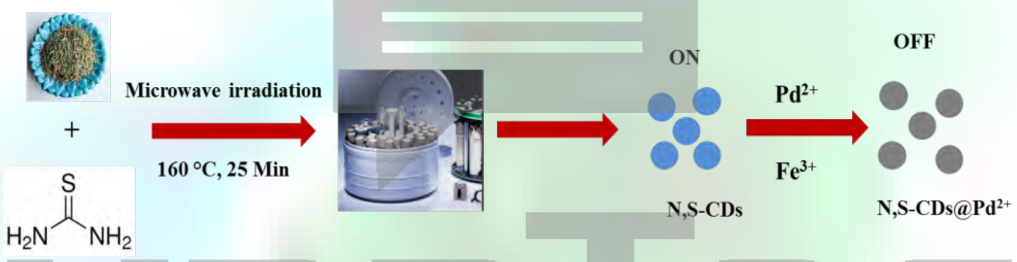
Graphical Abstract



Abstract: Iron is an essential transition metal for both plants and animals. However, it is potentially toxic to humans at excess concentration levels. Palladium (II) is also a transition element that plays an important role in cancer treatment, dental crowns, jewelry, and electronics [1]. Pd(II) is used as a catalyst for many reactions, and the contamination with Pd^{2+} requires extensive purification [2-3]. Thus, the determination of iron and palladium in environmental and biological samples is important and has been attracted much attention.

In this research, A fluorometric nanosensor is designed for the determination of Pd^{2+} or Fe^{3+} using nitrogen, sulfur carbon dots (N, S-CDs). The N, S-CDs were synthesized by microwave using thyme extract as the carbon source and thiourea as the nitrogen and sulfur source. The prepared N, S-CDs have the strongest excitation/emission peaks at 350/450 nm and a 53% fluorescence quantum yield. The N, S-CDs were employed as a fluorescent probe for the determination of Pd^{2+} with a linear response in the 0.1-120.0 µM concentration range with the limit of detection (LOD)

of 0.029 μM. The probe also responds linearly to Fe^{3+} in the 0.1-300.0 μM concentration range with a limit of detection of 0.025 μM. The probe was employed for the determination of Fe^{3+} in whole milk powder, serum, and urine samples.

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A 3D Printed Microfluidic Device in Combination with Smart-Phone-Based Colorimetric Detection for Field Analysis of Heavy Metals

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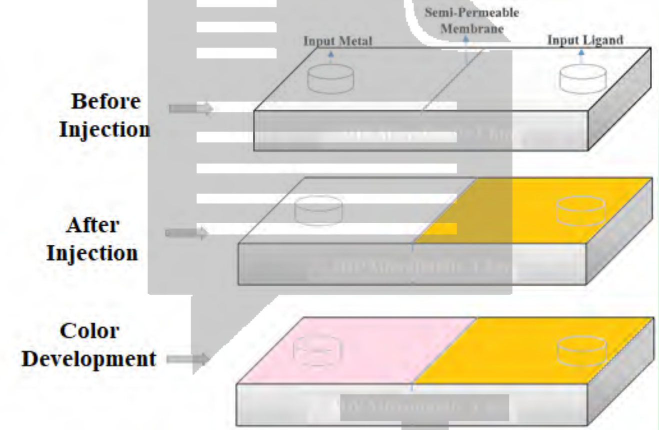
Graphical Abstract



Abstract: In the present work, a portable microfluidic chip was 3D printed and coupled with a smartphone-based colorimetric detection system and applied for field analysis of heavy metals (mercury and lead) in environmental water samples. The procedure was based on complex formation between heavy metal and dithizone ligand, on both sides of a porous membrane. The color intensity was graded using a smartphone, exploited as the detection and data processing system. Different experimental parameters affecting the analytical signal including acid concentration in sample solution, concentration of ligand, and contact time were studied and optimized using a multivariate optimization design. Under the optimum conditions, the method showed a linear dynamic range between 0.5 and 100 μg mL^{-1} with a determination coefficient of 0.9953. The limits of detection and quantification were obtained 0.1 and 0.3 μg mL^{-1}, respectively . The method provided a precise determination with relative standard deviations in the range of 4.1–

5.3% .The seutp was successfully applied for the determination of heavy metals in wastewater, and tap water samples with spiking recoveries in the ranges of 93–98%, and 89–97%, respectively.

Keywords: 3D printing, Microfluidic, Smartphone-based colorimetry, Heavy Metals

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Field Determination of Phosphate in Water Samples Using a 3D Printed Microfluidic Chip

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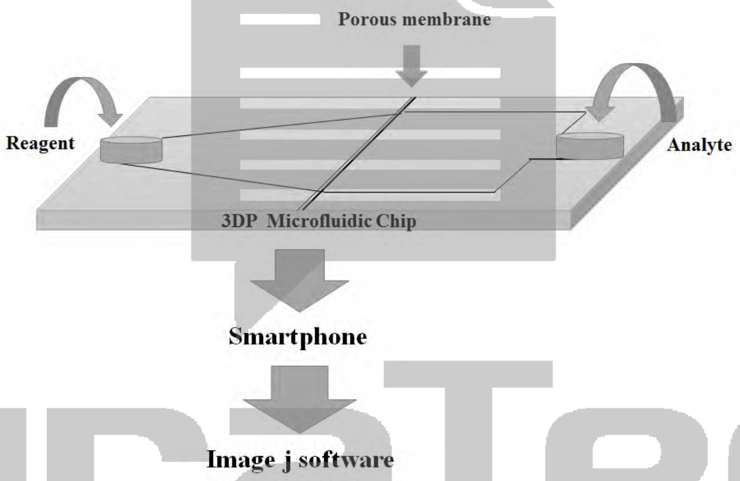
Graphical Abstract



Abstract: Phosphorus is one of the essential elements that is widely applied as a fertilizer in agriculture, as a detergent in industry and as a softener in water tretment, as weel as in beverage drink and food products to prevent the growth of mold and bacteria. However, it has diverse effects, especially when released into the aquatic environment, by reducing the level of water-soluble oxygen [1-4]. Thus, fast on-site analysis of phosphate in aquatic ecosystems is a vital inquiry. In this research, a simple and low-cost microfluidic device was 3D printed and uesed for field analysis of phosphate in environmental samples. An image-based colorimetric detection method was used based on the complex formation of phosphate ions with ammonium heptamolybdate. The influential experimental parameters including pH of sample, reaction time, and concentration of chromogenic reagent were investigated and optimized using a Box-Behnken design (BBD). The calibration curve was linear within 0.1-50 μg mL^{-1} (R^2> 0.996) of phosphate. Total time of each experiment was obtained 8 min. The microfluidic device was successfully applied for the determination of phosphate in real water samples.

Keywords: 3D printed microfluidic chip; phosphate; environmental samples; Box-Behnken design.

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Nitrogen-Doped Graphene as An Efficient Sorbent for Needle Trap Device

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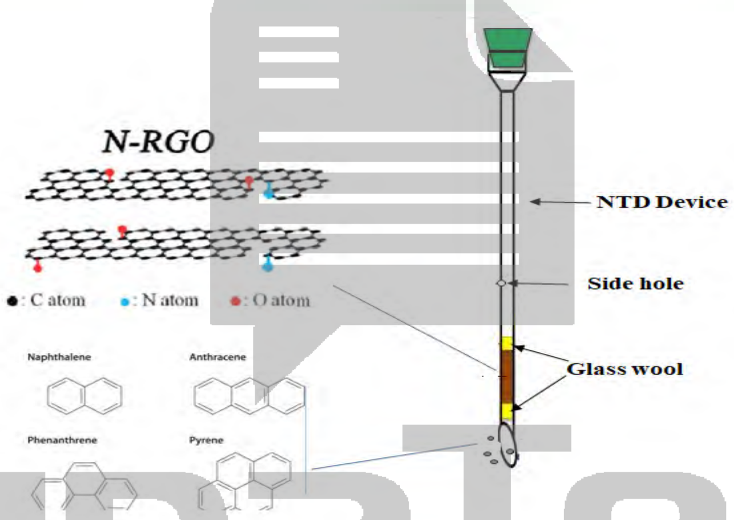
Graphical Abstract



Abstract: Less oxygen-containing functional groups in reduced graphene-oxide (RGO) compared to GO, increases the percentage of G-band (sp^2 carbon network), which leads to an increase in its affinity toward aromatic compounds, particularly polycyclic aromatic hydrocarbons (PAHs). This effect is significantly improved by doping RGO with nitrogen atoms, resulted in an increase in its adsorption capacity to PAHs. Herein, nitrogen modified reduced graphene oxide (N-RGO) was synthesized through a hydrothermal method and packed into a stainless-steel needle for preparation a needle trap device (NTD). The nanocomposite sorbent was characterized by SEM and FT-IR spectrometry. The N-RGO packed NTD was used for the extraction of PAHs from polluted soil samples, followed by GC-FID measurement. Different affecting experimental variables, including extraction temperature, flow rate, desorption time and desorption temperature

were studied and optimized using a multivariate optimization design. Under the optimal conditions, the calibration graphs showed good linearities ($R^2 > 0.99$) over the concentration range of 0.01-1.0 µg g^{-1} for naphthalene, 0.05-1 µg g^{-1} for phenanthrene, 0.02-1 µg g^{-1} for acenaphthene , 0.04-1 µg g^{-1} for fluoranthene, and 0.01-1 µg g^{-1} for pyrene. The limits of detection, limits of quantification and relative standard deviations were found to be in the ranges of 0.05-0.17 ng g^{-1}, 0.2-0.6 ng g^{-1} and 9.7-15.4% (n=6), respectively. Finally, the proposed NTD-GC-FID method was successfully applied for the extraction and determination of PAHs in contaminated soil samples.

Keywords: Nitrogen-Doped Graphene, Needle Trap Device, PAHs, GC-FID.

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Photocatalytic Aerobic Oxidation of Aliphatic Alcohols $CoFe_2O_4$/Ce-UiO-66 Nanocomposite

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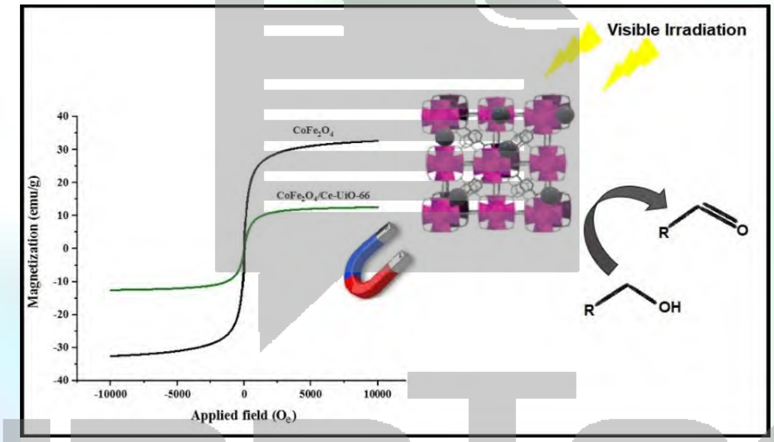
Graphical Abstract



Abstract: During the past years, light-driven selective oxidation of various alcohols has attracted increasing attention as a green and eco-friendly manner to convert visible light energy into valuable compounds. In this work, magnetic $CoFe_2O_4$/Ce-UiO-66 embedded structure composites is elaborately designed for the photocatalytic oxidation of aliphatic alcohols under visible-light irradiation and aerobic condition at room temperature. The catalyst showed high chemical stability in the reaction conditions and can be recovered quickly and reused for at least 5 reaction runs in the aerobic oxidation reaction condition.

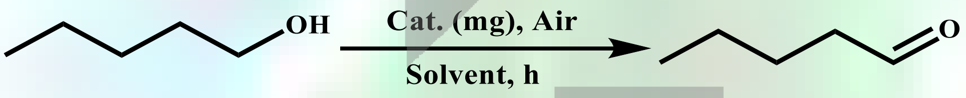
Metal-organic frameworks (MOFs) are crystalline porous compounds formed by metal oxo-clusters which, connected to polytopic organic linkers[1]This compounds have structural flexibility, tuneable pore size and, adjustable surface area. These MOFs could be employed in various fields such as gas separation and adsorption, sensing, drug delivery, catalysis, and electro/photocatalysts.

The crystal structure of the compound is built up by the 12-connected hexa nuclear clusters of $[Ce_6O_4(OH)_4]^{12+}$ with dicarboxylate (BDC^{2-}) linkers, ideal composition of $[Ce_6O_4(OH)_4(BDC)_6]$ [2].

MOF with other semiconductors such as spinel-type ferrites as magnetic materials and photocatalysts, resulting in enhanced chemical stability, recyclability and photocatalytic performance. the Co-ferrite/MOF structures reusable, owing to the possibility to use an alternative magnetic field for reviving the nanocomposite [3].

In this work, novel $CoFe_2O_4$/Ce-UiO-66 nanocomposites with superparamagnetic properties were successfully synthesized .The combination of $CoFe_2O_4$ and Ce-UiO-66 leads to a high photocatalytic activity for aerobic oxidation of aliphatic alcohols to the corresponding aldehydes under visible light irradiation. More significantly, the Co-ferrite/Ce-MOF nanocomposite can be easily removed from a reaction medium by adding an external magnetic field and able to reuse.

To conclude, oxidation of aliphatic alcohols to carbonyl compounds is of great interest for the production of industrial chemicals. Oxidation of aliphatic alcohols due to insufficient activity and low selectivity is more challenging than aromatic alcohols, which are readily transformed into aldehydes. Here we successfully prepared a magnetic composite of CoFe2O4/Ce-UiO-66 for demonstrated a general, convenient, green, and highly efficient principle for the photocatalytic aerobic oxidation of alcohols under visible light.



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Synthesis and Characterization of Fe_3O_4@SiO_2@SBA3-SO_3H for Paraquat Adsorption in Aqueous Solutions

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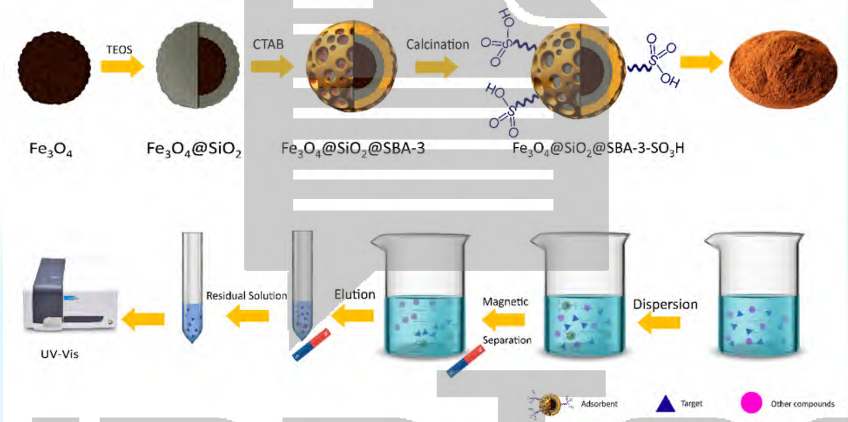
Graphical Abstract



Abstract: Paraquat (1,1-dimethyl-4,4-dipyridinium chloride), also known as methyl viologen, is one of the most widely used herbicides of toxicological class I in about 130 countries [1]. It is consideres as an effective herbicide in spite of its highly toxicity for humans and animals [2].

In the present study, a simple synthesis approach was applied to prepare the core-shell Fe_3O_4@SiO_2@SBA3-SO_3H mesoporous magnetic nanoparticles (MMNPs-SO_3H) as an effective sorbent for paraquat removal from the aqueous solutions. The characterization of MMNPs-SO_3H was done by XRD, BET, BJH, FT-IR, FE-SEM, VSM, EDX and TEM instruments. The effect of the influential experimental variables including solution pH, adsorbent amount, contact time and ionic strength at four levels were optimized in 50 mL solution containing 25 mg L^{-1} paraquat by Taguchi design method (OA_{16}). Based on the ANOVA results, ionic strength (80.69 %) recognized as the most important factor contributing to the removal efficiency of paraquat followed by

adsorbent mass (12.67%), pH of solution (3.52%) and stirring time (0.141%) .The replicate removal experiments at optimum conditions (sample volume = 50 mL, adsorbent dosage = 0.12 g, solution pH = 7, ionic strength = without salt addition, contact time = 30 min) confirmed good removal efficiency as 86.9 %. The four kinetic models for the paraquat adsorption on the MMNPs-SO_3H were investgated and according to the obtained results, the pseudo-second order kinetic model was known as the best kinetic model ($R^2 > 0.99$, $q_{e,cal} = 80.0$ mg g^{-1}) showing the diffusion appears to play a key role in determining rate of adsorption onto the porous adsorbent. Adsorption equilibrium data were investigated by Langmuir, Freundlich, Temkin, and Dubinin-Radushkevich isotherm models for explanation the adsorption systems at equilibrium. Thermodynamic study showed the temperature effects on the paraquat adsorption to obtain the thermodynamic parameters. The negative $\Delta H°$ and $\Delta G°$ values indicated the exothermic and spontaneous nature of paraquat sorption on the surface of MMNPs-SO_3H. The negative $\Delta S°$ shows a decrease in the randomness at the interface of solution-adsorbent with the progress of sorption process. The negative E_a confirmed the physisorption process by exothermic nature of adsorption process.

Finally, the applicability of the proposed adsorbent for adsorption of paraquat from real aqueous samples were investigated and satisfactory results were obtained.

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Efficient Non-catalytic Oxidation of 1,5-Dihydroxynaphthalene with Iodosylbenzene in Water and the Presence of Polyvinylpyrrolidone

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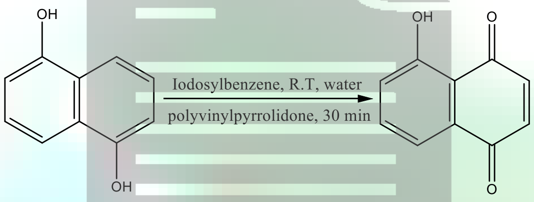
Graphical Abstract



Abstract: Non-catalytic oxidation of 1,5-dihydroxynaphthalene as an organic water pollutant phenolic compound to Juglone with iodosylbenzene in the presence of a water-soluble polymer and a short reaction time is reported.

Hypervalent iodine(III) reagents as environmentally friendly reagents have found many applications in oxidative transformations of organic compounds.[1] However, the polymeric structure of iodosylbenzene and most other hypervalent iodine(III) compounds, significantly decreases their reactivity towards the oxidation of organic substrates.[2] In continuing our studies on hypervalent iodine compounds, [3,4] herein the synthesis of a nearly water soluble analogue of iodosylbenzene from iodobenzene diacetate or pre-synthesized non-soluble iodosylbenzene in the presence of polyvinylpyrrolidone is reported. The oxidant was used as an efficient reagent for direct, quatitative oxidation of 1,5-dihydroxynaphthalene to Juglone in water, under mild conditions and a reaction time of ca. 30 min. UV-vis spectrophotometry at the λ_{max} of 1,5-dihydroxynaphthalene (301 nm, $\varepsilon = 7664\ M^{-1}cm^{-1}$) or Juglone (427 nm, $\varepsilon = 3811\ M^{-1}cm^{-1}$) was used for monitoring the progress of the oxidation reaction. It is noteworthy that in most of previous studies, the oxidation of organic compounds with iodosylbenzene was conducted using different transition metal complexes as the catalysts. [5-7]

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Design and Construction of Laboratory System to Treat and Reduce Wastewater Pollution in the Alcohol Industrytle

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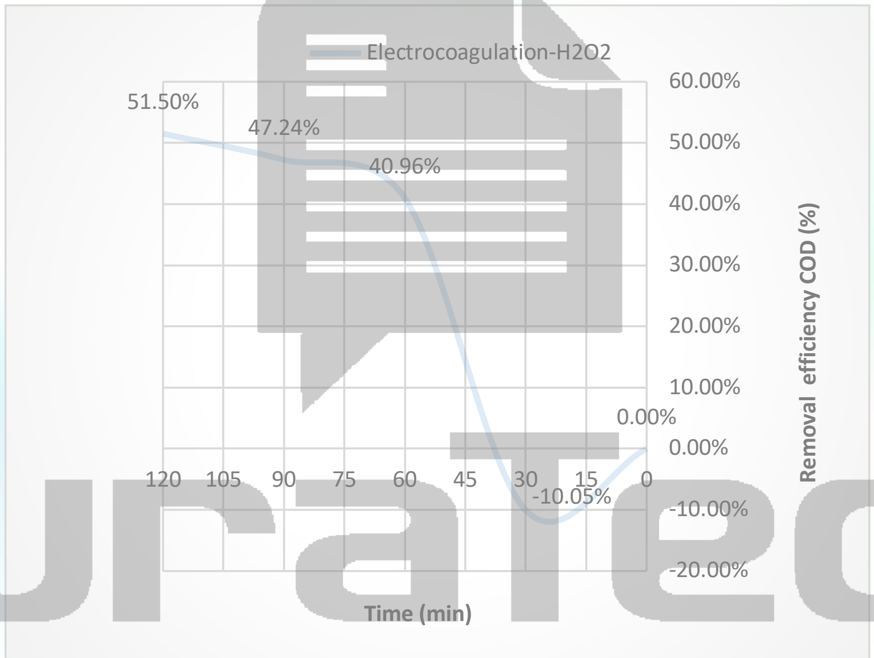
Graphical Abstract



Abstract: This Alcohol industry wastewater is an unwanted residual liquid waste that is generated during the alcohol production process and the resulting pollution is one of the major environmental problems. Despite standards for effluent quality, untreated or semi-treated effluents often pollute water sources. Alcohol distillation wastewater with its own unpleasant odor is a serious threat to water quality. The constant production of distilleries, on the one hand, and the strict legal regulations for the disposal of its wastewater, on the other, have necessitated the need to develop new technologies to create an efficient and economical process to improve the effluent flow of these factories[1]. One of the best and cheapest methods of industrial wastewater treatment is the

use of biological processes such as anaerobic reactors (UABR) and aeration reactors. But for alcoholic wastewater, due to the high percentage of organic and inorganic substances, the presence of aromatic toxins, especially phenols, stable brown color and low pH, the efficiency of aeration reactors due to high energy consumption and high oxygen consumption rate is very low. This process will still be dark, even if it results in significant removal of COD[2]. The color of melanoidins is hardly affected by conventional biological methods such as methane fermentation and activated sludge process[3,4], and it is very difficult to achieve ideal conditions in this type of reactor, but it seems that anaerobic processes if Properly designed, it can improve the chemical quality of Winas to some extent . Based on studies and experimental experiments, one treatment method alone is not effective and serialization of treatment processes improves the processes. In this study, by performing pre-treatment by chemical proxy electrocoagulation method, the effluent compounds of alcohol factories are converted into simpler compounds as much as possible to facilitate their biological decomposition and can be accepted in biological treatment plants. In designing and constructing a laboratory system, comparing the electrocoagulation and proxy electrocoagulation processes, as well as integrating the electrocoagulation prophylaxis process and 5 days anaerobic biological treatment, it was found that the combination of electrocoagulation and anaerobic proxies provides better results than other methods. .

In this process, with energy consumption of 24 kWh per cubic meter, the COD removal efficiency 62.1% and color removal efficiency 91.94% were obtained. Also the wastewater pH rose from 4.40 to 5.60. The effect of electrocoagulation proxy on TDS test parameter and electrical conductivity was not significant.

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Functionalized Organosilicate Materials as A Novel Fiber Coating In Headspace Solid Phase Microextraction Of Phthalate Esters

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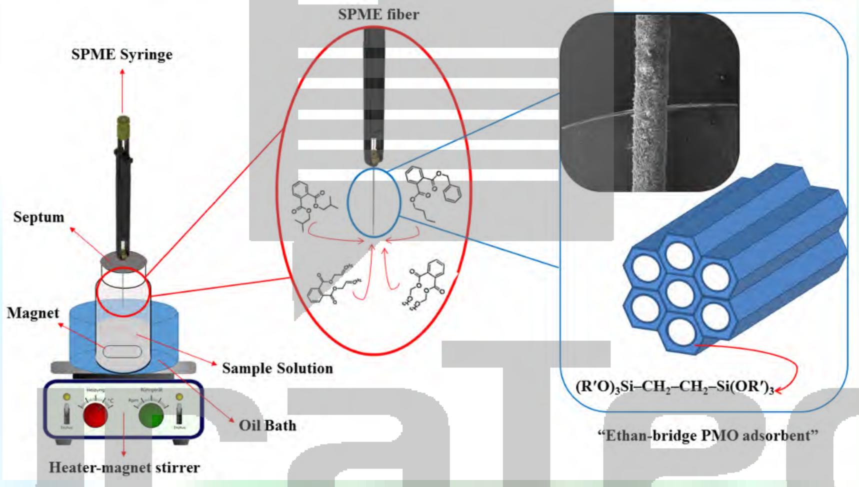
Graphical Abstract



Abstract: Sample preparation is common in many analyses and is developed to improve a specific analysis. This step may be the most time-consuming in analysis and affects significantly the analytical information [1]. Solid phase microextraction (SPME) was developed by Pawliszyn and his coworkers in the last decade. It has become an attractive sampling technique and gained widespread acceptance in many areas [2]. a new porous material was used as a coating in solid phase microextraction for extraction and determination of phthalate esters in complex matrices such as environmental and biological samples. The prepared nanomaterial was immobilized on a stainless steel wire for fabrication of the SPME fiber. The fiber was evaluated for the extraction of some phthalate esters from aqueous sample solutions and saliva in combination with the GC-FID

instrument. The extraction efficiency of SPME increases by using mesoporous silicas adsorbents due to its high surface area [3]. The resultant material was characterized by scanning electron microscopy, transmission electron microscopy, infrared spectroscopy, X-ray diffraction, and BET/BJH surface area/porosity, N_2 adsorption-desorption measurements. Key parameters affecting the extraction efficiencies, including extraction temperature, extraction time, ionic strength, and desorption temperature and time. Under optimum conditions, the repeatability for one fiber (n = 7), expressed as relative standard deviation (R.S.D.%), was between 4.8% and 8.7% for the extracted compounds. The limits of detection for the studied compounds were between 0.25 and 1 μgL^{-1}. The relative recovery was between 82 and 110%. The calibration curve was linear in the concentration range from 0.05 to 300 μgL^{-1}. The results showed suitable correlation coefficients (R > 0.99) for all of the analytes in the studied calibration range. The developed method offers the advantage of being simple to use, with shorter analysis time, lower cost of equipment, the thermal stability of fiber, and high relative recovery in comparison to conventional methods of analysis.

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Synthesis of Carbon-based Nanocatalyst with Dual Electrocatalytic Function for Ethanol Electrooxidation Reaction and Hydrogen Evolution Reaction

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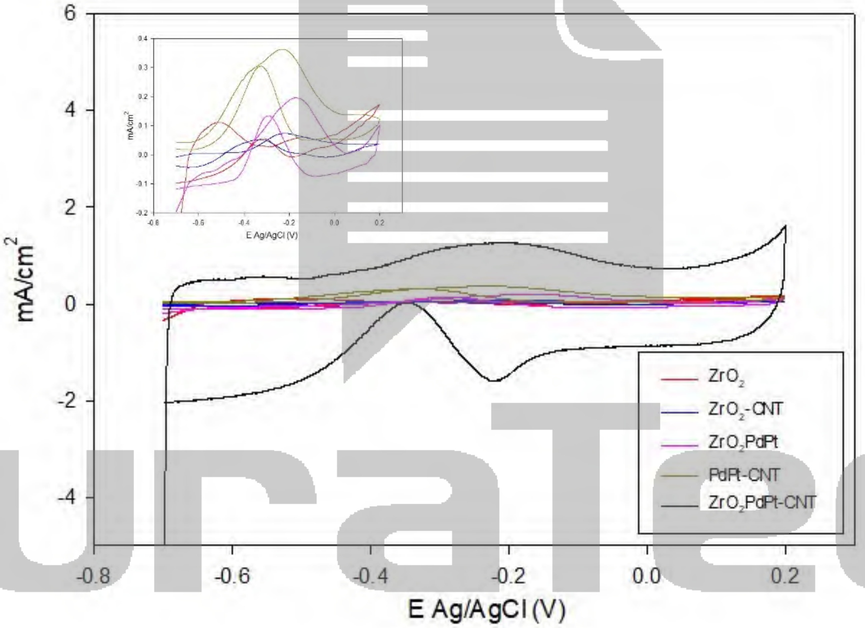
Graphical Abstract



Abstract: In recent decades, direct alcohol fuel cells have received much attention as a source of renewable energy. These cells can play an important role in replacing traditional fossil fuels, thus reducing the energy crisis and reducing greenhouse gas emissions. In this study, platinum and palladium with low load are used for ethanol electrooxidation reaction. Also, to improve the catalytic performance of ethanol electrooxidation, contact amplification and electron transfer, carbon and metal oxides supports were used simultaneously. The mechanism of oxidation and reduction electrode reactions was investigated by cyclic voltammetry electrochemical technique and catalyst activation by applying different potentials and a constant time of 300 seconds by chronoamperometry technique in alkaline medium. The results showed that the interaction of platinum and palladium and support can increase electron and mass transfer. This carbon-based catalyst was able to exhibit dual electrocatalytic performance for the ethanol electrooxidation

reaction and the hydrogen production reaction. The well-controlled morphology of Pt and Pd-based catalysts helped existing active surfaces and sites to be useful for catalytic processes.

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Application of Metal-Organic Framework and Sulfur Functionalized Graphene Oxide Composite as the Sorbent for Solid-Phase Extraction of Lead before its Determination by Flame Atomic Absorption Spectrometry

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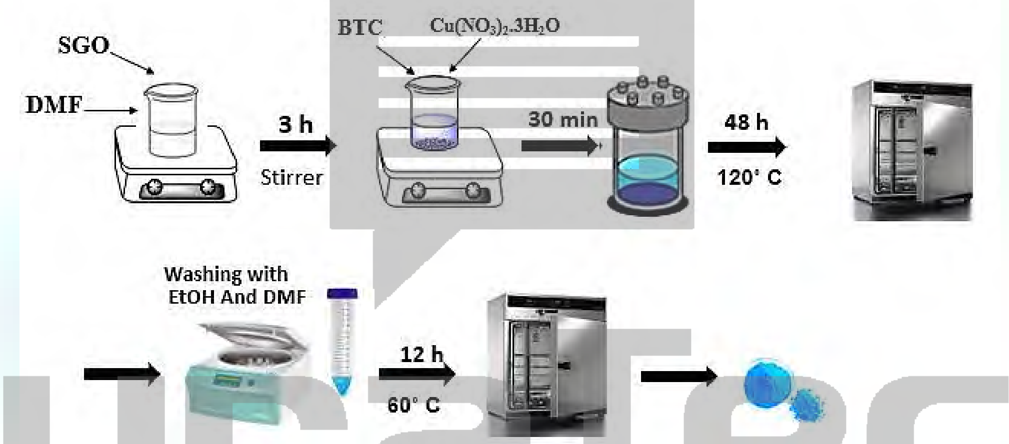
Graphical Abstract



Abstract: Lead is a highly toxic element for humans and other living organisms. Lead can cause great damage to the kidneys and brain and can interfere with the production of red blood cells [1,2]. Therefore, the determination of small amounts of lead in different samples is very important. The most common technique for measuring lead is flame atomic absorption spectroscopy. However, direct determination of the low concentration of this element in real samples is often not possible due to the low sensitivity and disturbance of the sample tissue with this technique and requires a separation and pre-concentration step [3].

This study describes the synthesis, identification, and application of a new composite including a metal-organic framework and sulfur functionalized graphene oxide as the sorbent for solid-phase extraction and preconcentration of Pb^{2+} ions from aqueous samples. The preconcentrated analyte was determined by flame atomic absorption spectrometry. The prepared sorbent was characterized using Fourier transform infrared spectroscopy (FT-IR), field emission scanning microscopy (FESEM), X-ray diffraction (XRD), and nitrogen adsorption and desorption isotherm (BET analysis). The effect of important parameters such as the sample pH, amount of sorbent, extraction time, sample volume, and type, concentration, and volume of the eluent on the extraction of the analyte was investigated and optimized. At the optimal conditions, the calibration graph was linear in the concentration range of 5.0-140.0 µg L^{-1} lead ions with a determination coefficient (R^2) of 0.9998. The limit of detection (LOD) and the limit of quantification (LOQ) of the method were 1.1 and 3.5 µg L^{-1}, respectively. The relative standard deviations (RSDs) of 1.5 and 2.1% were obtained at 12 µg L^{-1} concentration level of Pb^{2+} (n = 6) for intra- and inter-day analysis, respectively. The developed method was successfully employed for the determination of lead in different water and food samples.

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Investigation of Methanol Electrooxidation on Metal Alloy Catalysts

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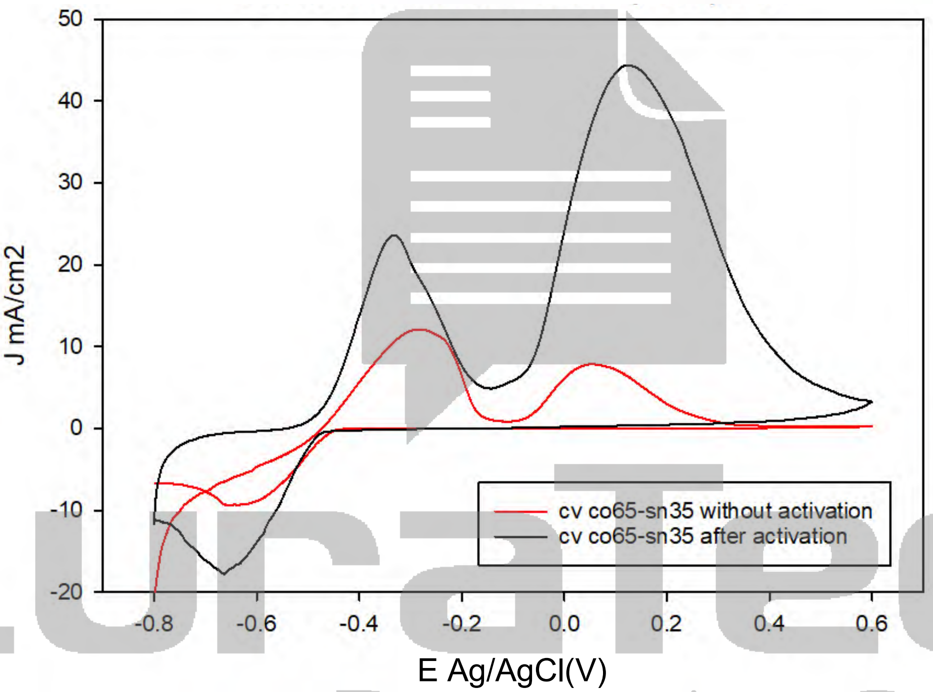
Graphical Abstract



Abstract: Direct methanol fuel cells have been considered for their simple and convenient configuration for small and portable applications. One of the issues that has challenged the practical use of fuel cells as a safe and environmentally friendly tool is the improvement of the catalysts and nanocatalysts used in them. In this study, an innovative method of in-situ cathodic electrochemical activation to increase the electrocatalytic activity of metal alloys in the methanol electrooxidation reaction in acidic and alkaline media has been investigated. The alloys used in this study are free of platinum and palladium as two precious catalysts. In the present study, a cyclic voltammetry technique was used to investigate the electrocatalytic activity of alloy nanoparticles in methanol electrooxidation. The voltage range selected for the acidic environment

was -0.8 to 0.6 volts and for the alkaline environment -0.1 to 0.7 volts according to the reference potential with a scan rate of 50 mV/s. The results showed that the use of metal alloys along with in-situ cathodic electrochemical activation will increase the electrocatalytic activity in the methanol electrooxidation reaction in both acidic and alkaline media.

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Removal of Cadmium from Aqueous Solutions Using Modifed Saffron Corm Tunics as Biosorbent

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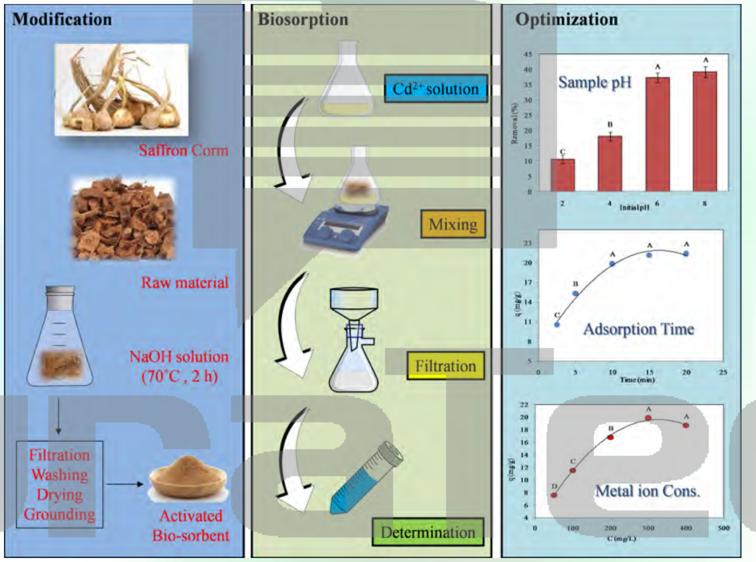
Graphical Abstract



Abstract: Recently, biosorption using agricultural waste materials has emerged as the most promising and viable method, with advantages of high adsorption capacity and no detrimental effects on the environment [1, 2]. Pretreatment with dilute sodium hydroxide solution has been the most popular method of improving surface properties and removing soluble organic components of plant wastes applied for biosorption [3]. Saffron (*Crocus sativus* L.) corm tunics is an agricultural waste, which has been studied for its potential application as a biosorbent. Surface modification was carried out in NaOH solution at 70˚C for 2 h. The results showed that the adsorption process was highly dependent on the adsorbent dosage and Cd^{2+} initial concentration. A sample pH 6.0-7.0 was favourable and, Kinetic data were fitted well to the pseudo-second-order

model with R^2=0.997 and q_{max}=25.64 mg g^{-1} at the initial concentration of 50 mg L^{-1}. The Langmuir isotherm model was best applicable for obtaining the equilibrium parameters with R^2=0.999, K_L= 0.072 L mg^{-1}, and q_{max}= 20.11 mg g^{-1}. The negative values of ΔGº imply that the adsorption of Cd^{2+} was a spontaneous and favourable process at temperatures below 40˚C. The ΔHº is also negative, revealing the exothermic nature of the process. These results demonstrate that saffron corm tunics are effective, environmentally friendly, and low-cost biomaterial for Cd^{2+} removal from aqueous solutions.

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A Selective Colorimetric Chemosensor for Determination of $C_2O_4^{2-}$, In Aqueous Solution Based on ArsenazoIII-Cu Complex

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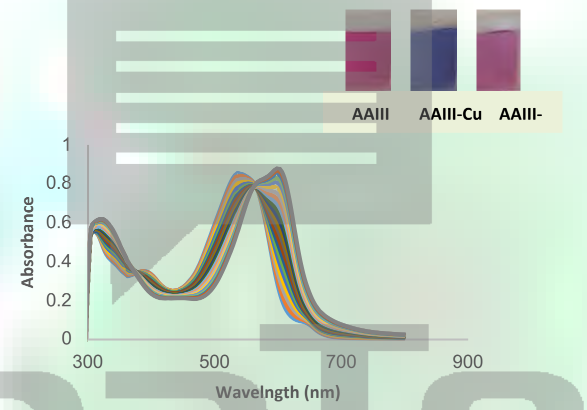
Graphical Abstract

AAIII – Cuرسم نمودار جذب بر حسب طول موج کمپلکس



Abstract*:* An-spectrophotometric approach is described for the determination of $C_2O_4{}^{2-}$ ion in the aqueous medium based on the formation of ArsenazoIII(AAIII) –Cu complex. This system produces a visible color change from red to blue based on the indicator displacement assay (IDA) method due to formation AAIII-Cu complex by addition of Cu^{2+}ion. In the presence of $C_2O_4^{2-}$ ion, the solution color returns to red with about 34.5 nm blue shifts. Determination of $C_2O_4^{2-}$ ion the linear ranges achieved for UV-Vis absorbance experiment were 1.5 - 47 µmolL^{-1}. The limits of detection was also achived to 0.23µmol L^{-1}. Anion species various such as SO_4^{2-}, $S_2O_8^{2-}$, $H_2PO_4^{2-}$, CH_3CO^{2-}, CN^-, $S_2O_4^{2-}$, SO_3^{2-}, PO_4^{3-}, HPO_4^{2-}, CO_3^{2-}, NO_3^-, SCN^-, I^-, Br^-, Cl^- and F^- were investigated by AAIII –Cu complex. This complex no indicated spectral and color changes with these species. The method was applied to the determination of oxalate ion in aqueous solutions samples.

Keywords: Colorimetric, chemsensor, ArsenazoIII –Cu complex, $C_2O_4^{2-}$ ion

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Colorimetric Chemsensor Based on ArsenazoIII for Determination and Naked-Eye Detection of Argenin in Aqueous Solutions

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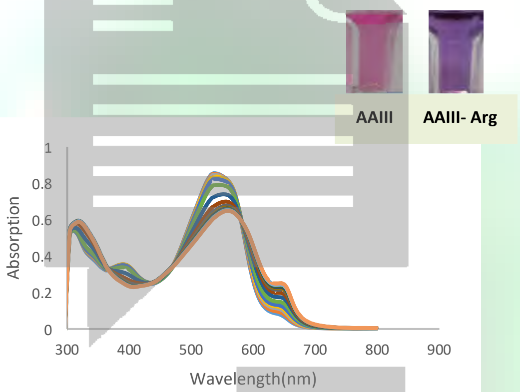
Graphical Abstract

رسم نمودار جذب برحسب طول موج AAIII



Abstract: Arginine (Arg) is a semi-essential amino acid in humans that plays an important role in maintaining balance hormones, strengthening the immune system, wound healing and tissue integrity. Excessive amounts can cause allergies, loss of consciousness, low blood pressure and swelling of the limbs Therefore, determining Arg and knowing the proper intake of this amino acid is essential for maintaining human health. In this paper, spectrophotometric and colorimetric method for the determination of Arg in aqueous medium using ArsenazoIII (AAIII) is described. Adding Arg to AAIII as chemosensor causes a visible color change from red to purple and decrease of absorbance at 536 nm which related interaction between of AAIII and Arg. The linear dynamic range was achieved for UV-Vis absorbance experiment were 15-340 μmolL^{-1}. The limits of detection was also calculated to 0.04 μmolL^{-1}. This method was employed for the determination of Arg in environmental samples which gave satisfactory results.

Keywords: Colorimetric chemsensor, ArsenazoIII, Argenin

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Carminic Acid as a Green Colorimetric Chemosensor for Sensitive and Selective Determination of Bismuth(III) in Biological Samples by UV–Visible Spectrophotometry

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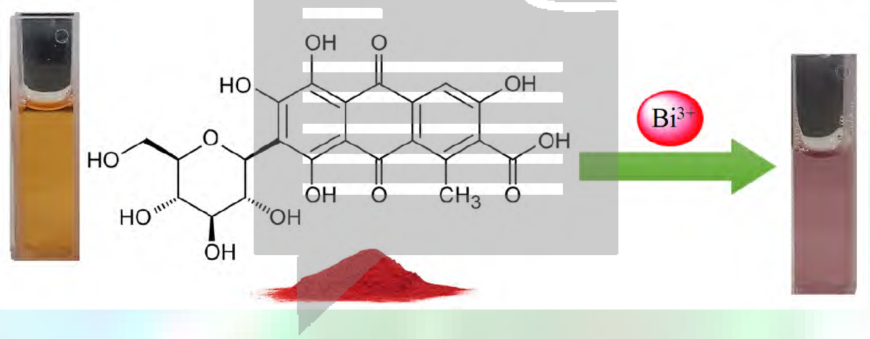
Graphical Abstract



Abstract*:* At present time, fluorescent and colorimetric chemosensors because of simplicity, less time-wasting, portability and cheapness have been attending as efficient tools for the detection of numerous metal ions such as bismuth [1]. Unfortunately, most of these chemosensors are synthesis organic compounds, which are harmful to man and the environment [2]. Carminic acid (CA) is an incredibly stable and reliable natural dye and doesn't have any specific health and environmental risks [3]. In this study, we introduced a new colorimetric chemosensor based on carmine dye for sensitive and selective determination of bismuth ions in buffer solution with pH 4. According to the method detection limit is 0.056 μmolL^{-1} and linear dynamic ranges between 0.40 to 46.59 μmolL^{-1}. No serious interference was evaluated during analysis of at least 100-fold excess of various cations species such as Ni^{+}, Fe^{3+}, Ag^{+}, Pb^{2+}, Al^{3+}, Zn^{2+} Mg^{2+}, Ce^{3+}, Co^{2+}, Cu^{2+}, Mg^{2+}, Mn^{2+}, Cr^{3+}, Ca^{2+}, Na^{+}, K^{+}, Hg^{2+}, V^{5+}, NH$_4^{+}$, Ba^{2+}, Sr^{2+}. The suggested method was applied for the determination of bismuth in various human plasma samples.

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Electrofenton Process Based on Iron Electrodes for The Removal of Ponceau 4R from Aqueous Solutions

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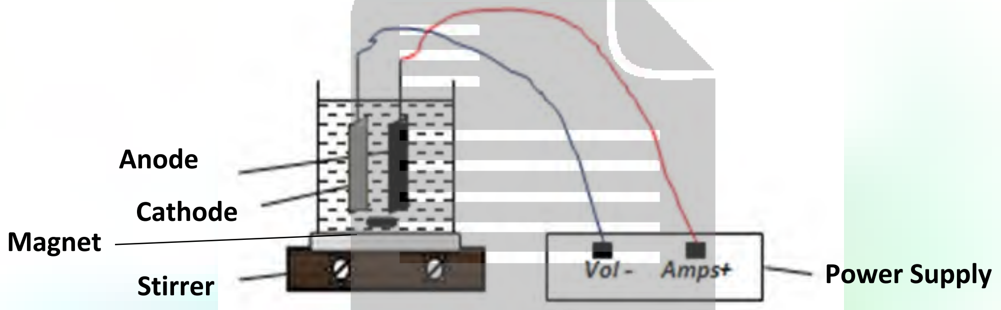
Graphical Abstract



Abstract: The dye compounds could be hazardous to human's health. Ponceau 4R known as Acid Red 18 or E124 is a water-soluble azo dye with acidic group that widely used in the food industry and drug products. Due to its disadvantage on human health, the removal of Ponceau 4R from wastewaters is important before its entrace to the environment [1]. The aim of this study was to remove Ponceau 4R by electrofenton process using iron electrodes from aqueous solutions. In the electrofenton process, the continuous electrogeneration of H_2O_2 is achieved by O_2 reduction in the presence of dissolved Fe^{2+} by different reduction processes [1]. For electrofenton process, a glass reactor with a total volume of 900 mL containing two iron electrodes (63 × 80 × 2 mm) was used. This set up was connected to a power supply. The effect of five effective parameters such as applied voltage (5, 10, 15, 20 V), ionic strength (0, 0.05, 0.1, 0.2 M), dye concentration (50, 100, 200, 250 mg L^{-1}), pH of solution (2, 3, 4, 6) and percentage of H_2O_2 (10, 20, 25 ,30 %) were investigated in four levels and optimized by Taguchi orthogonal array design method (OA_{16}). The residual concentrations of Ponceau 4R after electrofenton process was spectrophotometrically determined (505 nm) in the time range of 0-90 min with time intervals of 10 min and the removal

efficiencies were obtained. Based on the results, the optimum conditions were obtained as pH: 4, voltage: 20 V, H_2O_2: 25%, salt concentration (Na_2SO_4): 0.05 M and the initial concentration of dye: 50 mg L^{-1}. Under the optimum conditions about 100 % of Ponceau 4R was removed during 20 min.

The results confirmed the eclectrofenton process is able to remove Ponceau 4R with maximum efficiency at a short time.

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Removal of Disulfine Blue from Aqueous Solutions Using Electrofenton Process: Optimization by Taguchi Orthogonal Array Design

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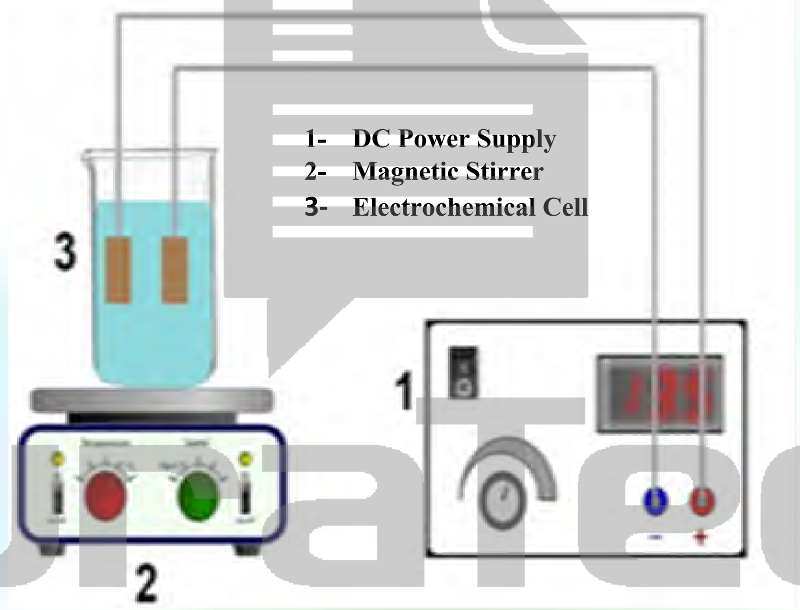
Graphical Abstract



Abstract: Synthetic dyes are used for coloring many different products such as textiles, paper, cosmetics and drugs [1]. Disulfine blue is a synthetic dye that has been widely applied in different industries including coloring paper, temporary hair colorant, dyeing cottons, wools and so on. In spite of its applications and advantages, it can cause some illnesses for humans. So, its removal from water resources is still a vital task [2]. The advanced oxidation processes (AOPs) constitute an attractive approach due to the high oxidation potential of hydroxyl radicals, their non-selective nature and the possibility of rendering full mineralization of a wide variety of organic pollutants. The electrofenton process is the most common AOP processes based on Fenton's reaction, which

enhances the degradation of organic compounds with generated hydroxyl radicals. In electrofenton, H_2O_2 is continuously supplied to a contaminated acidic solution by the two-electron reduction of injected O_2 at the cathode, whereas Fe^{2+} ion is added to react with this species to generate Fe^{3+} ion and •OH in the bulk from Fenton's reaction, which is mainly propagated by the cathodic reduction of Fe^{3+} ion to Fe^{2+} ion [3].

The purpose of this work was to study the degradation of Disulfine blue dye by electrofenton process. In the present study, an electrofenton glass reactor (900 mL) equipped with two iron electrods (63 × 80 × 2 mm) and a power supply was constructed for removal of Disulfine blue from polluted waters. The effects of affecting experimental parameters including applied voltage (5, 10, 15, 20 V), ionic strength (0, 0.05, 0.1, 0.2 M), dye concentration (50, 100, 200, 250 mg L^{-1}), pH of solution (2, 3, 4, 6) and percentage of H_2O_2 (10, 20, 25 ,30 %) were investigated using Taguchi orthogonal array design method (OA_{16}). The residual concentration of Disulfine blue after electrofenton process was determined using UV-Vis spectrophotometer at wavelength of 639 nm in the time range of 0-90 min with time intervals of 10 min and dye removal efficiencies were obtained. Based on the results, the optimum conditions were obtained as pH: 2, voltage: 20 V, H_2O_2:10 %, salt concentration (Na_2SO_4): 0.1 M and the initial concentration of dye: 50 mg L^{-1}. Under the optimum conditions, more than 99 % of Disulfine blue was removed during 50 min. The results confirmed the eclectrofenton process is able to remove Disulfine blue with maximum efficiency at a short period of time.

Reference

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Modified Hollow Fiber Membrane with Silver/Multiwall Carbon Nanotube/Polyaniline Nanocomposite as a Sensing Element for Voltammetric Measurement

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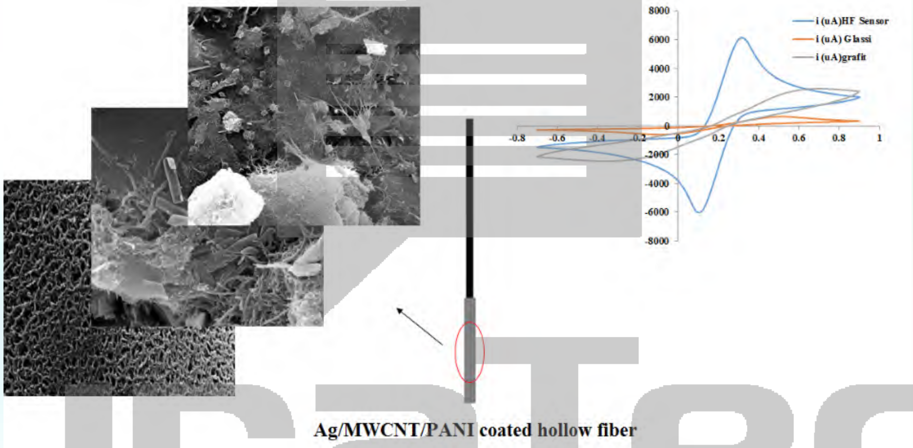
Graphical Abstract



Abstract: Electrochemical techniques are powerful analytical techniques that used successfully for determination types of pharmaceutical samples. These techniques are simple, effective, low-cost and reliable with high sensitivity, accuracy, precision and wide linear dynamic range [1]. Carbon-based sensors have been extensively used in the electrochemical studies. Carbon nanotubes are suitable for electrodes preparation due to their high electrocatalytic activity, high chemical stability and low fouling. In addition, multiwall carbon nanotubes (MWCNTs) are widely applied as the appropriate modifiers in preparation of some electrodes because of their ability to improve the facility of electron transfer between electro-active species and electrodes [2, 3]. In this research, the hollow fiber membrane was modified with silver/multiwall carbon nanotube/polyaniline (Ag/MWCNT/PANI) nanocomposite by electrophoretic deposition (EPD) method and used as the sensor for voltammetric measurement of dipyridamole (DIP) in aqueous solution. The surface morphology and electrochemical properties of the electrode was evaluated by SEM, TEM, EDX, XRD and EIS. The electrochemical efficiency of the proposed electrode was investigated with cyclic voltammetry (CV) and differential pulse voltammetry (DPV) techniques for determination of DIP in aqueous solution. The limit of detections (LODs) and linear dynamic ranges (LDRs) for DIP were obtained 0.001-50 μM and 1.0×10^{-3} μM, respectively. The sensor was successfully employed to determine DIP in real samples such as pharmaceutical formulations.

Keywords: Electrochemical sensor; Hollow fiber membrane; Ag/MWCNT/PANI nanocomposite; pharmaceutical products; DIP; EPD.

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Effect of Time on the Removal of Pb(II) Heavy Metal Ion by $[Ca(H_2btec)\cdot H_2O]_n$

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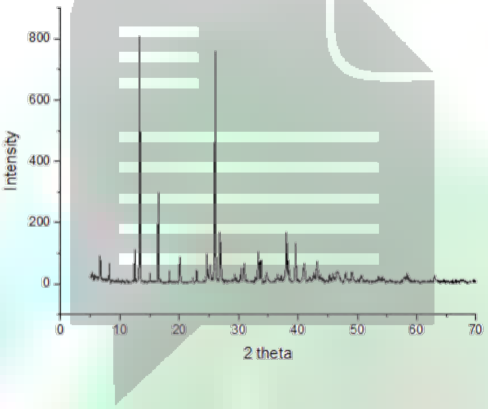
Graphical Abstract



Abstract: Among the water pollution sources, heavy metals are considered as the most hazardous, because of high toxicity to human health and badly damage the kidneys, brain and nerves as well as causing birth defects [2]. Based on the promising feature of MOFs they could act as a favorable candidate for heavy metal removal applications [3]. The calcium-based metal-organic framework synthesized by the deposition method using benzene-1,2,4,5-tetrakis carboxylate linker. Characterization of MOF was performed using XRD, SEM, and FTIR analyses [1]. The MOF has then applied to efficient adsorption of Pb(II) pollutant ions. Contact time as one of the different effective parameters was investigated. Adsorption capacity of 50 ppm was obtained for this adsorbent in less than 15 minutes. The potential of adsorbent $[Ca(H_2btec)H_2O]_n$, btec: benzene-1,2,4,5-tetracarboxylic acid was investigated by the adsorption and desorption cycles in three steps. Desorption process was carried out via adding $[Ca(H_2btec)H_2O]_n$ to the solution containing Pb(II) ions. After ultrasonic bath. The adsorbent was seprated by centrifugation and the residual ion was measured using ICP-AES.

Keywords: Ca-MOF, Adsorption, Pb(II), pollutant

Reference

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Electrochemical Investigation of Rosmarinic acid in the Leaf Extract of *Melissa officinalis L.* at the Surface of Silver Nanoparticles Modified Carbon Paste Electrode

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Abstract: Rosmarinic acid (RA) is one of the flavonoid species which is abundantly found in fruits and vegetables. Importance of RA has attracted attention of scientists, and anti-inflammatory, antioxidant, antitumor, anti-viral, anticancer and antibacterial effects of it have been reported by many of scientists [1]. Statistical analysis indicated that in *Melissa officinalis L.* extract, rosmarinic acid is at the highest level [2]. On the other hand, electrochemical methods are widely applied to the study of the reactions of catechol species. RA has two electroactive catechol moieties, which are independent of each other and can participate in the electrochemical oxidation-reduction process [3]. In this work at first the biosynthesis of silver nanoparticles has been performed with the leaf extract of melissa officinalis L. Synthesized nanoparticles were confirmed by UV-Visible and FT-IR spectrophotometer, XRD and SEM image. Silver nanoparticles, with large surface area, good biocompatibility, high conductivity and electrocatalysis characteristics, have been suitable for facilitate the transfer of electrons at the carbon paste electrode (CPE) [4]. In the second step, we constructed a novel, stable and sensitive electrochemical electrode based on silver nanoparticles, paraphine and graphite, as the working electrode for the electrooxidation of rosmarinic acid. Electrochemical and adsorption behaviour of rosmarinic acid at the surface of this modified electrode investigated using cyclic voltammetry and differential pulse voltammetry techniques at the biological pH.

Keywords: Electrochemical oxidation; Rosmarinic acid; Silver nanoparticles; Modified carbon paste electrode.

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Electrochemical Oxidation and Assessment of Antixidant Activity of Aquouse *Artemisia Absinthium L.* Extract

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Abstract: Electrochemical evaluations are useful for the determination of antioxidant activity for example, their application as a rapid evidence of the antioxidant capacity of many organic compounds. The oxidation potentials measured by cyclic voltammetry (CV) used to compare the antioxidant strength of phenolic acids, flavonoids, cinnamic acids as natural compounds in medicinal plants. [1] On the other hand, it is clear that medicinal plants used in the traditional medicine and healing are one of the sources of antioxidants. The dietary intake of antioxidants plays an important role in the protection of the human organism against free radicals. Free radicals or reactive oxygen species generated by our body by various endogenous systems by exposure to different physiochemical conditions or pathological states. In the normal condition and for proper physiological function, a balance between free radicals and antioxidants is necessary [2]. *Artemisia absinthium L* .is an important perennial shrubby plant that has been widely used for the treatment of several ailments. Traditionally, A. absinthium has always been of pharmaceutical and botanical importance and used to manage several disorders including hepatocyte enlargement, hepatitis, gastritis, jaundice, wound healing, splenomegaly, dyspepsia, indigestion, flatulence, gastric pain, anemia, and anorexia. [3]. In the present work the electrochemical oxidation of *Artemisia absinthium L.* extract has been investigated by cyclic voltammetry and differential pulse voltammetry techniques in the biological pH at the surface of glassy carbon electrode at various concentrations and scan rates. The results revealed that the extract had an irreversible redox reaction. Also our results show that *Artemisia absinthium L.* extract oxidize at low potentials in comparison of quercetin, gallic acid and salicylic acid as a standard antioxidants. Antioxidant activities of this extract was evaluated using the 2,2-diphenyl-2-picrylhydrazyl (DPPH) radical-scavenging method and it is directly related to its redox potential value. The results show the good antioxidant activity of the *Artemisia absinthium L.* extract and the electrochemical behavior of the constituents in it, at the surface of glassy carbon electrode.

Keywords: Electrochemical oxidation; Antioxidant activity; *Artemisia absinthium L.* extract.

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Improved Aqueous Lead Adsorption by Using Sand@MOF Composite

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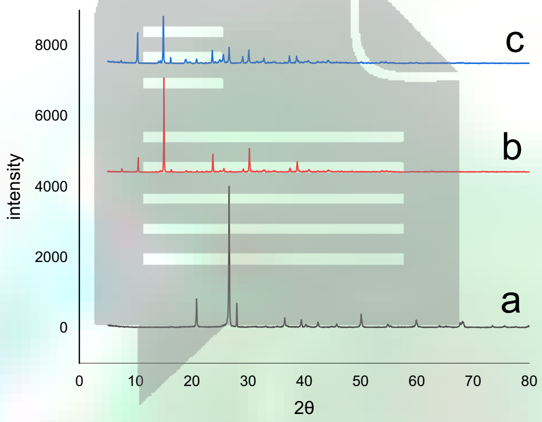
Graphical Abstract



Abstract: Among the most common pollutants in industrial effluents are various types of heavy metal pollutants that reducing the amount of them in water is necessary. Metal Organic frameworks (MOF) are among the porous materials that can be used to absorb heavy metals [1,2]. We report here a work in which a MOF with the formula of $\{[Ba_2(H_2btec)\cdot H_2O]\cdot 0.5H_2O\}_n$ (btec is benzene-1,2,4,5-tetracarboxylic acid) was applied to absorb lead [3]. In effect, the composite of this porous MOF with a sand sample containing silica which is also a porous material, has increasingly improved lead absorption. Many analytic methods including SEM, XRD, and FTIR were applied to characterize the composite and its constituents. However, XRD patterns of a) sand, b) MOF c) composite of sand and MOF illustrate the good formation of the composite. Investigating the concentration of lead in the initial solution compared with its concentration in the final solution after adsorption on sand, MOF and composite shows that Pb ion is adsorbed better on the composite with a meaningful difference.

Keywords: Ba-MOF, Sand, Composite, Adsorption, Lead

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A Novel Nanostructure-based Genosensor for Detection of *Shigella dysenteriae* in Human Plasma Samples by Porous MoS_2 Nanosheets and Au Nanoparticles

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Abstract: *Shigella dysenteriae (S. dysenteriae)* is a species of the rod-shaped bacterial genus *Shigella*. *Shigella* species can cause shigellosis (bacillary dysentery). The most commonly observed signs associated with *Shigella dysentery* include colitis, malnutrition, rectal prolapse, tenesmus, reactive arthritis, and central nervous system problems. Further, *S. dysenteriae* is associated with the development of hemolytic-uremic syndrome, which includes anemia, thrombocytopenia, and kidney failure. If infected with S. dysenteriae, an individual will experience a severe case of shigellosis. Most cases of shigellosis are in developing countries. Shigellosis outbreaks in Asia, Latin America and Africa have had mortality rates of up to 20%. Due to negative effects of the *S. dysenteriae* in human health, highly-sensitive determination of this pathogenic agents is of great importance. In this study, electrochemical oligonucleotide genosensor based on DNA hybridization process was developed to detect *Shigella dysenteriae* in human plasma samples. The porous MoS_2 nanosheets were initially casted on the electrode. Then, Au nanoparticles (AuNPs) was electro-deposited on the electrode surface. The obtained modifier agent was effectively used for electrochemical analysis of the bio-assay. Various electrochemical techniques including cyclic voltammetry (CV) and Differential pulse anodic stripping voltammetry (DPASV) have been used to investigate the applicability of the fabricated genosensing bio-assay. Under optimal conditions, LOD were calculated 9.14 fM. In addition, a wide linear range was obtained. The fabricated bio-detection assay indicated high selectivity for 1, 2, and 3 base mismatch sequences and also high recovery indexes in human plasma samples. In addition, a negative control of the biosensing platform was provided. The obtained results

confirmed that the biosensor possess high selectivity. Moreover, the RSD% (relative standard deviation) was below 5 which indicated the high accuracy and repeatability of the sensing assay.

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Synthesis and Characterization of Hybrid Silica Aerogel and Its Magnetic Nanocomposite Material

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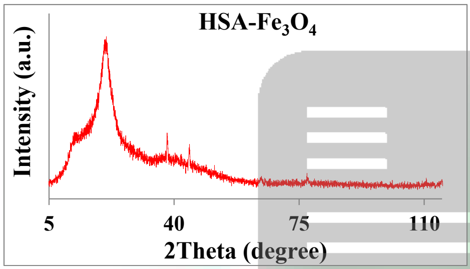
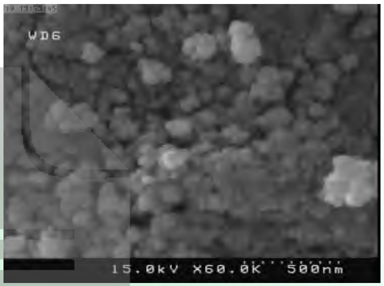
Graphical Abstract





Abstract: Aerogels are porous inorganic polymers having high porosity, low density, high specific surface areas, low refraction index in addition to very little thermal conductivity [1]. Due to their exceptional properties, they have found numerous advanced applications [2]. They are typically synthesized via common sol–gel chemistry and subsequent supercritical drying procedure in order to prevent destroying the porous structure by capillary stress [3]. The sol–gel synthesis includes hydrolysis catalyzed by acid or base and then silicon alkoxides condensation. Silica aerogels are achieved by atmospheric pressure drying technique in which both of the network strengthening as well as surface modification happen before the drying stage [4,5]. Herein, hybrid silica aerogel (HSA) nanoparticles were synthesized by sol-gel method and drying at ambient pressure. Also, a magnetic nanocomposite of HSA with Fe_3O_4 nanoparticles (HSA-Fe_3O_4) was prepared. The morphology, structure and magnetic properties of the HSA as well as its nanocomposite were analyzed by SEM, XRD, VSM and ATR-FTIR techniques. The saturation magnetization (M_s) values for the Fe_3O_4 NPs, and HSA-Fe_3O_4 nanocomposite film were 69.93, and 19.04 emu g^{-1}, respectively. The XRD pattern of the Fe_3O_4 NPs exhibited the standard peaks at 2θ values near 30, 35, 43, 53, 57 and 63° related to the crystallographic planes (220), (311), (400), (422), (511) and (440) matched the JCPDS card No. 75-1069. The HSA illustrated a broad peak centered at around 19.91° signifying its amorphous nature. The XRD pattern of the HSA-Fe_3O_4 NPs was similar to that of the HSA but the Fe_3O_4 NPs peaks were observed due to the presence of higher amount (70 w/w%) of HSA in the HSA-Fe_3O_4 NPs composite.

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Activity Evaluation of Co/Zn-NC@PPy-800 as a Non-noble ORR Catalyst in Fuel Cell-based Breath Ethanol Sensor

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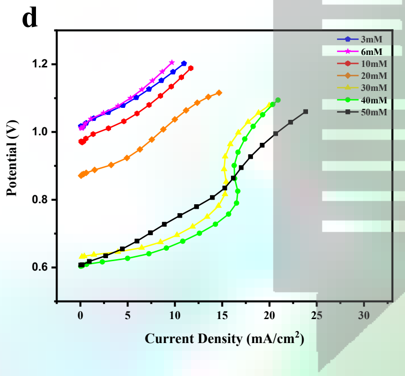

Fig1. (a) T EM image of Co/Zn-NC@PPy-800

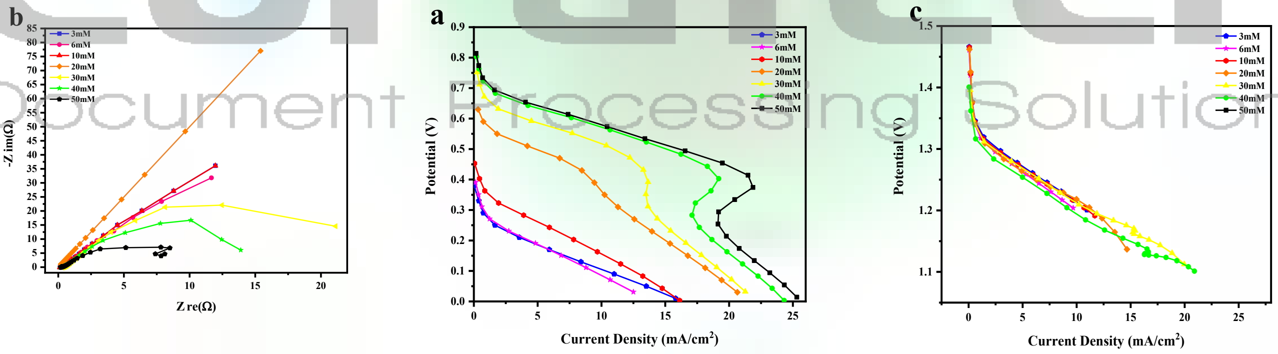

Fig2. (a) DEFC polarization curve, (b) Nyquist plot of DEFC, (c) Cathode and (d) Anode polarization. Fuel and oxidant: ethanol solution (3mM to 50 mM) and air, Cell temperature: room temperature, oxidant pressure: ambient.

Abstract: The oxygen reduction reaction (ORR) plays a leading role in electrochemistry. The ORR is one of the most challenging issues in many types of electrochemical instruments such as Lithium-air batteries and fuel cell-based breath alcohol sensor (BrAS). The challenge is the slow ORR kinetics and its essential need for Pt-based catalysts; These issues have led to attempt to substitute Pt-based catalysts with nonprecious metal catalysts (NPCs). In this work, Co/Zn-NC@PPy-800 is used as an ORR catalyst. According to the Fig. 1, the nanostructure of Co/Zn-NC@PPy-800 is made up of approximately equally formed N-doped sheet-like carbon (Fig.1a). The cell performance evaluation is depicted in Fig. 2. The cell is made of 60 wt. % Pt/C with loading of 10 mg. cm^{-2} and Co/Zn-NC@PPy-800 with loading of 2 mg. cm^{-2} as anode and cathode electrocatalysts, respectively. The anion-exchange membrane (A201 Tokuyama), with a thickness of 28 µm is used as electrolyte. The fuel is fed using various concentrations of 3 mM – 50 mM of ethanol in a 2 M KOH solution. The cell polarization curves (Fig. 2a) demonstrate that with decreasing in ethanol concentration, decreasing in current and power density will occur. This behavior exhibits changing of response against changing of concentration and it is suitable for alcohol sensor applications. Electrochemical impedance spectroscopy (EIS) experiments represent increasing the diameters of semicircles with decreasing in the concentration of ethanol (Fig. 2b). Cathode and anode polarizations are displayed in Fig. 2c and Fig. 2d respectively and it can be found that cathode polarization is constant in various concentrations of ethanol, which means changing ethanol concentrations do not affect cathode polarization. In contrast, anode polarization has a direct relation to ethanol concentration and lower fuel concentration lead to more anode polarization due to more fuel mass transfer limitation.

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Acute Toxicity of Different Ag Nanoparticles Based on Their Physicochemical Properties with The Aid of Chemometrics

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Abstract: Nanoparticles are particles that have dimensions of 1 to 100 nanometers and in all three dimensions. Materials in the nanoscale have exceptional contrasting properties to that of similar materials in bulk. These distinctions are due to the basic and physical properties of metal molecules and surface to volume proportion to nanotechnology progression. The most important advantage in nanomaterials is the increase in surface area and reactivity by reducing the size [1]. However, high toxicity of NPs for living organisms is a strong limiting factor that hinders their use. The swift rise in the popularity of using nanomaterials for new products has not been overlooked by the manufacturers of environmental cleanup tools. Evaluation is required to understand possible adverse effects and their fate inside the human body and environmental cleanup [1,2]. Knowledge of different properties and toxicity is necessary before any use of nanoparticles and in order to safely use . Measurement of physicochemical properties such as size, shape, surface charge and number of nanoparticles controls their toxicity. Reaction with organic ligand and conversion of metal core and change of surfaces to modify nanoparticles affect their toxicity [3-6].

In this study, classification of 94 different Ag NPs based on their physicochemical properties like primary size, Primary hydrodynamic diameter, DLS Hydrodynamic diameter in the test media and zeta potential was done. The respons of data were their acute toxicity in different organisms including Daphnia magna, Thamnocephalus platyurus, Escherichia coli K12, Pseudomonas fluorescens OS8, Saccharomyces cerevisiae, Pseudokirchneriella subcapitata, Murine fibroblast and Bacillus subtilis BR151. This classification was done by statistical methods including PLS-DA and kohenen maps . The accuracy of applied method in classification of nanoparticles was more than 80%.

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Cd(II) removal from Water Using Magnetic Hybrid Silica Aerogel Nanocomposite Adsorbent

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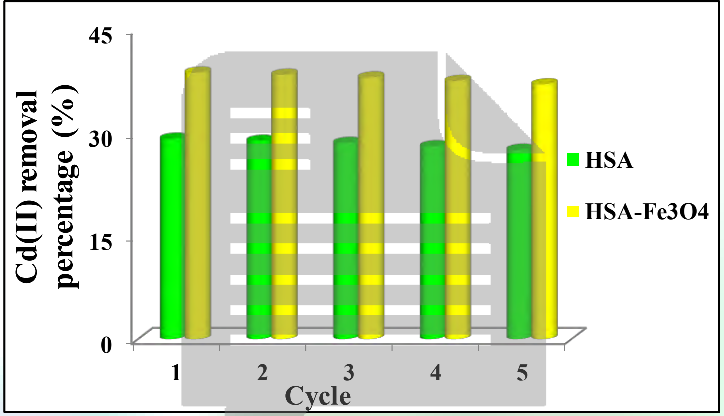
Graphical Abstract



Abstract: Heavy metal contamination is a serious ecological worldwide problem which is progressively enhanced by developing the industrial activities [1-3]. Cadmium (Cd) is one of toxic heavy metals that can be entered into surface waters and soils in concentrations significant to human health through industrial wastes [4]. The increasing environmental existence of cadmium is primarily caused by its application in stabilizers, phosphate fertilizer, ceramics, alloys, pigments, electroplating plants and battery [5]. The abilities of the hybrid silica aerogel (HSA), and HSA-Fe_3O_4 adsorbents were assessed for removal of cadmium(II) heavy metal ions (100 ppm) from aqueous solution. All adsorbents removed/adsorbed the maximum Cd(II) ions in 120 min when adsorbent dosage=20 mg and pH=8. Moreover, the highest adsorption capacities were 58.5, and 65.8 mg/g for the HSA, and HSA-Fe_3O_4, respectively. Kinetic studies using all adsorbents verified that Cd(II) adsorption obeyed the second order model illustrating the analyte chemisorption was happened on the adsorbents surfaces. All adsorption data were well consistent to the Langmuir isotherms. The reusability experiment confirmed that all of adsorbents could preserve >95% of their initial adsorption capacities even after five series of adsorption/desorption tests.

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Neutral red as Novel and Highly Selective Chemosensor for Detection and Determination of Cyanide in Aqueous Media

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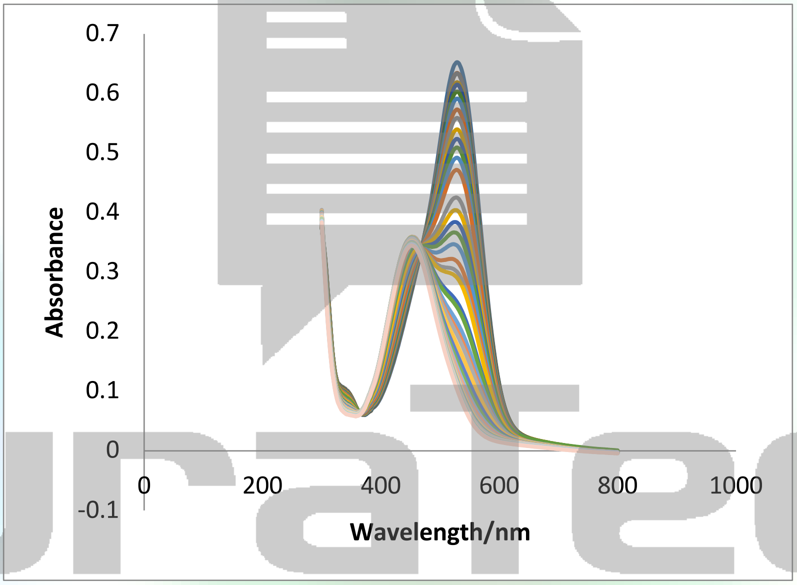
Graphical Abstract



Abstract: Anions play important role in chemical, biological and environmental processes. An important aspect of modern chemistry is the utilization of hydrogen bonding in the development of receptors for recognition of anions [1]. Among various anions, cyanide is one of the most concerned anions because it is highly toxic and harmful to human health since cyanide binds to the ferric form of cytochrome-c and inhibits the mitochondrial electron-transport chain [2]. There are several limitations associated with many of currently available cyanide sensors: such as (i) These sensors work only in organic solvents; (ii) They have poor selectivity over fluoride or acetate; (iii) They show low sensitivity; and (iv) They possess short-wavelength absorption or

emission [3]. Anion receptors are that reported rather difficult to synthesize or require expensive instruments for detections. Taking this dilemma into consideration recently, we have undertaken an extensive research program to explore bromopyrogallol red as an easily available dye demonstrated a high chromogenic receptor for cations and anions [4]. In this work, we disclose a new approach toward this goal. Neutral red (NR) actualized the novel and simple chemosensor for cyanide concept in water media. The binding sites of the receptor are directly attached to binding of anions could be monitored by changes in the photophysical properties of the receptor by UV–Vis spectroscopy and naked-eye detection. Neutral red has been identified as highly sensitive probe for CN^- which responds at 0.2 μmol L^{-1} concentration levels among other competing anions through a fast response time of less than 40 s which is much lower than most recently reported chromogenic probes. This method could have potential application in a variety of cases requiring rapid and accurate analysis of CN^- for human serum and water samples.

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Electrocatalytic Oxidation of Methanol on Gold Electrode Modified by Gold-Platinum Nanoparticles Dispersed into Ag/Halloysite Nanocomposite Film

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Abstract: Fuel cells which are the energy converting devices with a high efficiency have been attracting more attention in recent years due to high-energy demands, fossil fuel depletions and environmental pollution throughout the world [1]. Platinum has been used as the most popular catalyst in fuel cells for many years. However, pure Pt is much cost and it can be poisoned by CO intermediates which are produced during methanol electrooxidation [2]. In order to improve the activity of methanol electrooxidation, a common strategy is alloying Pt with other metals, such as PtIr, PtSn and PtRu [3,4].

In the present work, halloysite/AgNPs/ Pt –Au nanocomposite was used as an effective and novel catalyst for electrooxidation of methanol. At first, a certain amounts of halloysite and AgNPs suspensions were dropped onto the surface of the gold electrode. Then, the surface of the electrode was coated with platinum and gold (Pt –Au) nanoparticles through cyclic voltammetry technique. The surface of the modified electrode was then characterized by scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDX) techniques. In addition, the effects of various parameters such as methanol concentration, amount of the Ag nanoparticles and number of scan cycles of the Pt –Au nanoparticles electrodeposition on the electrooxidation of methanol were investigated and they were optimized. The electrooxidation of methanol on the surface of the modified electrode was studied using cyclic voltammetry and chronoamperometry. The obtained results show that proposed catalyst has a high electrocatalytic activity towards the methanol electrooxidation reaction as compared to Pt catalyst.

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Design a Novel Colorimetric Chemosensor for Selective Detection and Determination of Carbonate ion Based on Phosphotungstic acid Complexes of Neutral red in Water Media

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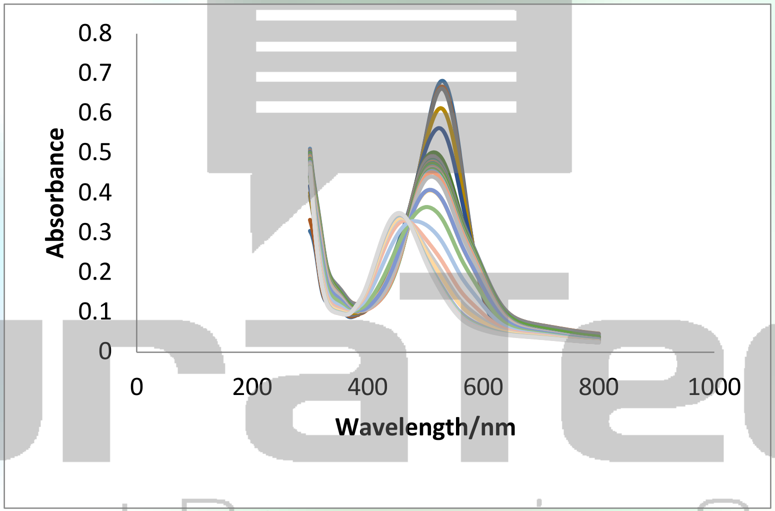
Graphical Abstract



Abstract: Carbonate is one of the onions that is only slightly toxic, but large doses are corrosive to the gastro-intestinal tract where symptoms may include severe abdominal pain, vomiting, diarrhea, collapse and death [1]. Colorimetric sensing which invariably bank on “naked-eye “sensing, has gained additional impetus owing to the ease in monitoring of the process without resorting to sophisticated techniques. Thus a great deal of effort has been invested in developing simple-to-make and use “naked-eye “diagnostic tools for sensing of analytes [2, 3]. These receptors are rather difficult to synthesize or require expensive instruments for detections. Taking this dilemma into consideration recently, we have undertaken an extensive research program to explore bromo

pyrogallol red as an easily available dye demonstrated a high chromogenic receptor for cations and anions [4, 5]. In this work, we disclose a new approach toward this goal. We manifest a novel neutral red (NR) based colorimetric chemosensor for carbonate ions in aqueous media. The phosphotungstic acid (PTA) binding property of NR was studied by the use of UV– Vis spectrophotometry and the attended color changes allowed assessment of the complex property of NR. Initial experiments aimed at the optimization of concentration of PTA led us to treat aqueous solution of CO_3^{2-} with NR-PTA formed in solution. Spectrophotometric monitoring of the changes revealed that the peak at 646 nm increased instantaneously with concomitant color change, because CO_3^{2-} is a strong p-acceptor. In order to support the above hypothesis, the process was repeated using scaled up quantities which unequivocally establish the proposed mechanism. The complex of NR-PTA also displayed ability to detect up to 0.18 μmol L^{-1} for CO_3^{2-}. This method could have potential application in a variety of cases requiring rapid and accurate analysis of CO_3^{2-} for real samples.

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Fabrication of Polyether Sulfone / Kappa-carrageenan Composite Membranes to Remove Tetracycline from the Aqueous Medium and Improve their Performance by Adding Ionic Liquids

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Abstract: Today, industries and industrial plants are the largest consumers of water, which in turn produce large volumes of wastewater. Industrial wastewater, in other words, is a by-product of manufacturing plants. In this research, membrane filtration method for industrial wastewater treatment has been used to treat wastewater containing tetracycline drugs available in the pharmaceutical industry. Membranes with different weight percentages were synthesized from polyether sulfone (PES), Aliquat 336 ionic liquid and kappa-carrageenan, so that the properties of these membranes were investigated by SEM, FT-IR and contact angle analyzes. PWF and tetracycline removal percentage by fabricated membranes were also evaluated. The results of SEM images showed that the irregular membrane structure of the membrane with ionic liquid increased with the addition of kappa-carrageenan polymer, the membrane structure was very regular and the flow rate of the membrane increased. However, the percentage of membrane clogging due to the presence of kappa-carrageenan polymer and the presence of hydrogen groups on the membrane surface and the formation of hydrogen bonds with tetracycline molecules increased the clogging of PES membrane. The highest volume of water leaving the membranes was related to PES-0.5A-0.5 membrane. The highest percentage of tetracycline removal according to the results of UV analysis was reported for samples collected from membrane tuberculosis related to PES-0.5A-1C membrane with 98% removal percentage, which is the highest removal percentage without change in flux Had a passage. The results of contact angle for fabricated membranes showed that adding ionic liquid and kappa-carrageenan biopolymer did not have much effect on the contact angle of PES membrane. The best contact angle of membranes made with 60.88 ° angle was related to PES-0.5A membrane. The results of FT-IR analysis showed that all bonds related to PES polymer appeared in the fabricated membranes. The only bond that appeared to contain the Aliquat336 ionic fluid with the PES polymer in the fabricated membranes was the CH_2 tensile bond.

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Development of Nanocomposite Anticancer Drug Delivery System Based on Chitosan by Molecular Dynamics Simulations

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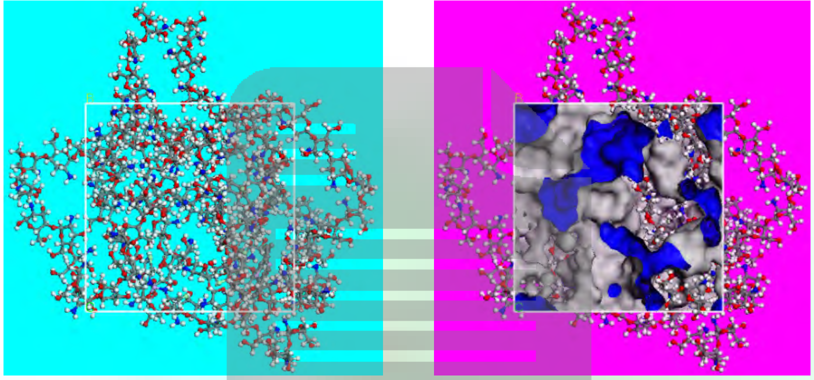
Graphical Abstract



Abstract: Cancer is known as one of the leading causes of human mortality which results in almost 13% of human death [1]. Even though numerous efforts are being made to advance the cancer therapies, number of new cancers is still increasing [2]. In order to increase the biocompatibility of graphene and its derivatives in biomedical applications, its composites with different polymers are usually prepared. Among diverse biopolymers, chitosan (CS) has drawn attention in pharmaceutical and biomedical applications due to its bioavailability, mucoadhesivity, biocompatibility, biodegradability, non-toxicity and low-immunogenicity [3,4]. The capacity of chitosan (CS) nanocomposite system containing graphene (G), nanoparticles for the delivery of ifosfamide (IF) anticancer drug was examined by means of molecular dynamics (MD) simulations in order to find a suitable drug delivery system (DDS). The kinetic, potential and non-bond energies of CS-G-IF were nearly 2020, 4810 and 5160 kcal/mol, respectively. The bulk density of the CS-G-IF matrix was obtained equal to 1.2914 g/cm^3. The free volume (FV) of the CS-GN-IF system was measured to be 11465.68 Å^3. The fractional free volume (FFV) is the ratio of FV to the entire volume of the cell. It was observed that CS-GN-IF had the FFV of 39.9154%. The surface areas of CS-G-IF was equal to 7853.84 Å^2. An appropriate drug diffusion coefficient was achieved for the CS-G-IF (0.0693×10^{-5} cm^2/s) which verified the IF diffusion in the CS-GN-IF was controllable and could cause an effective drug delivery.

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Temperature Influence on The Drug Delivery Performance of Chitosan Nanocomposites: A Molecular Dynamics Simulation Study

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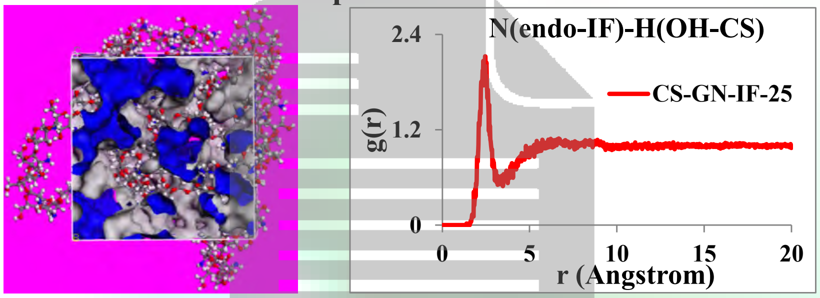
Graphical Abstract



Abstract: The classical cancer therapies such as chemotherapy are unfortunately ineffective due to their side effects, poor cellular uptake and drug resistance. Therefore, it is necessary to design and develop new drug delivery systems (DDSs) to decrease these drawbacks and enhance efficiencies [1]. A DDS is a formulation, dosage form or device that can introduce a drug into the body to improve its efficacy and safety through controlling drug release rate/place [2]. Chitosan (CS) is a natural cationic polysaccharide which is frequently used as drug delivery system due to its outstanding characteristics [3]. Molecular dynamics (MD) simulations are broadly accomplished to understand physical phenomena occurring in complex membranes at the molecular level [4]. In this work, molecular dynamics (MD) simulations were carried out on chitosan nanocomposite systems containing N-doped graphene (GN) or P-doped graphene (GP) nanoparticles for the delivery of ifosfamide (IF) anticancer drug in order to find the most suitable DDS. Moreover, the effect of temperature on the characteristics of these systems was investigated by running the MD simulations at four temperatures (298.15, 308.15, 318.15 and 328.15 K). The mean square displacement (MSD) and diffusion coefficient were enhanced by increasing the temperature. The surface area was enhanced by increasing the temperature from 298.15 to 328.15 K in the nanocomposites. It was recognized that at 298.15 K, the free volume (FV) was greater in the CS-GN-IF (11465.68 Å^3) whereas it was decreased to 11296.71 Å^3 in CS-GP-IF nanocomposite. Also, the FV was enhanced by raising the temperature from 298.15 to 328.15 K. A greater diffusion coefficient was measured at 328.15 K for the CS-GP-IF (0.0613×10^{-5} cm^2/s) but the CS-GN-IF revealed a lower diffusion coefficient (0.0565×10^{-5} cm^2/s) approving drug diffusion in the CS-GN-IF was more controlled leading to more efficient drug transport.

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Reformation of Hydrogen Electrolyser in Power Plant for Twofold Generation Hydrogen & Ozone

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Abstract: Hydrogen production via electrolysis of water from alkaline aqueous electrolytes is a valid typical technology [1,2,3]. Electrochemical hydrogen compression is seen as a promising alternative to mechanical compression in the context of power-to gas plants. It can be carried out either as direct co-compression in a water electrolyser or via a separate electrochemical hydrogen compressor . The Water electrolyser uses electrical energy to split water into oxygen at the anode and hydrogen at the cathode[2,4]. Hydrogen indirectly cooled stator of generators in the thermal power plant[3]. in addition, most electrochemically generated hydrogen is produced using alkaline electrolysers in a wide range of production processes, including the food industry for increasing saturation in oils and fats, their melting points and resistance to oxidation. and the nuclear industry requires H_2 for removing O_2 as it can cause stress corrosion cracking and power stations use H_2 as a coolant for its generators due it its high thermal conductivity. Oxygen, normally generate a by-product of electrolysis[4]. The generic reaction which takes place in a water electrolyser is: ($H_2O \rightarrow \frac{1}{2} O_2 + H_2$)

But by change in anode of electrolyser we can generate ozone instead of oxygen , Ozone is an environmentally-friendly oxidant that is widely used for industrial applications, such as water disinfection, air purification, and medical use [5].commercially available technology for ozone generation is based on electrochemistry (water electrolysis: $3H_2O \rightarrow O_3 + 6H^+ + 6e^-$) [6]. This approach can be achieved by suitable choice of the anode material to have a high over potential for OER and available couple with cathode to hydrogen generation. 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-PbO_2, Pt, Pt composites, boron-doped diamond, TiO_2 thin films on Si/TiO_x/Pt substrate, and Ti/Ni-Sb-SnO_2 catalysts are among the materials that have been used for EOP.[5-9] In this work, a high-performance porous titanium oxide electrode (Ti/TiO_2/Ni-Sb-SnO_2) has been developed for electrochemical production of ozone .The Ti/TiO_2 electrode was prepared using

anodizing method at high voltage for forming a layer of porous TiO_2 on the surface of Ti mesh, then followed by depositing a layer of Ni-Sb-SnO_2 under deep eutectic solvent on the Ti/TiO_2 surface. The deep eutectic solvent was used for electrodepositing, because its great effect on electrode performance. Ozone was electro generated from tap water or alkaline electrolyte on Ti/TiO_2/ Ni-Sb-SnO_2 electrodes at different operating conditions. Higher efficiency of O_3 generation was obtained at 3 V in alkaline electrolyte (Fig. 1).other electrode only with acidic electrolyte exponent to ozone generation but These electrodes were used in electrochemical ozone production (EOP) carried out during the electrolysis of electrolyte-free water or alkaline electrolyte in order to obtain an environmentally friendly technology for water treatment .

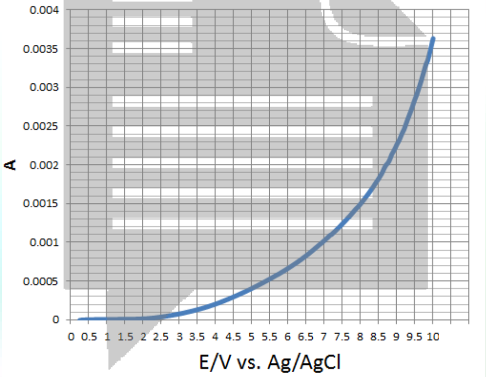

Fig. 1: Anodic linear sweeps at a scan rate of 50 mV/ s in alkaline electrolyte at 25◦C E (V) vs. Ag/AgCl/KCl (sat)

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MnO_2/Zeolite as A New Synthetic Nanocomposite for The Desulfurization of Thiophene

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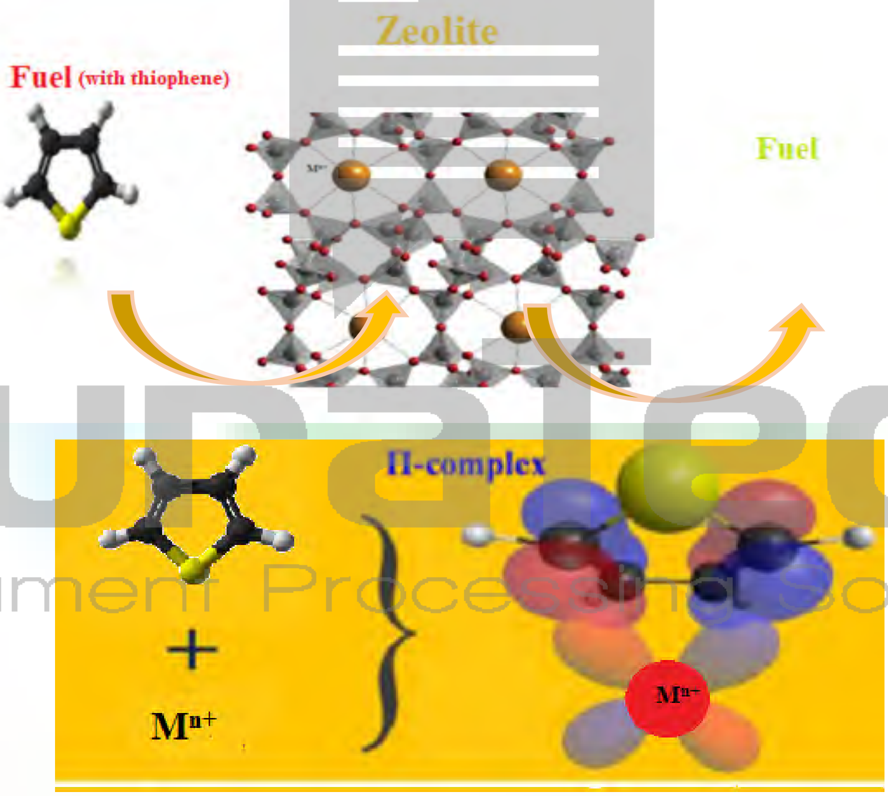
Graphical Abstract



Abstract: Over the past years, production of clean fuel has become an important issue from an environmental point of view. To obtion such clean fuel, we studied the role of adsorption/oxidation of MnO_2/zeolite nano composites under mild conditions. Zeolites with porous structure are very

promising in adsorption/removal of various componds. Also manganese dioxide (MnO_2) with different crystallographic forms (hollandite (α-MnO_2), pyrolusite (β-MnO_2), ramsdellite (γ-MnO_2), akhtenskite (ε-MnO_2), birnessite (δ-MnO_2) and nsutite (λ-MnO_2)) has attracted considerable attention due to high catalytic activity, facile synthesis, etc [1, 2]. In this work, birnessite (δ-MnO_2) with layer structure was prepared by the reaction of permanganate with $H_2C_2O_4$ at 363 K, and dried at 375 K [3]. Then MnO_2/zeolite nano composites were prepared by solid-state disperssion (SSD) methode. Different types of zeolite (Y, Fe-modified clinoptilolite (FeZ) and Cu-modified clinoptilolite (CZ)) were employed as supports for δ-MnO_2 nanoparticles and their catalytic activity were investigated in the adsorption/oxidation of thiophene from a model fuel at 298K. The samples were characterized by X-ray diffraction (XRD), infrared spectroscopy (FT-IR) and Scanning Electron Microscopy (SEM). The XRD analyses confirmed the formation of pure tetragonal structured δ- MnO_2. The average diameter was found to be 18.1 nm according to the Scherer equation. The catalytic activity of nano composites increased in the order of $MnO_2/CZ < MnO_2/Y < MnO_2/FeZ$. It is anticipated that the adsorption of thiophene takes place via the π-interaction between the adsorbent and thiophene molecules. Actually formation of π-complex between various sulfur and nitrogen containing compounds, olefins and π- electron-rich componds with adsorbent is a common process [4]. The employment of higher contents of MnO_2 (from 0.05g to 0.1g) in nano composites decreased the removal effeciency of thiophene.

Fuel, zeolite, MnO_2, thiophene, catalytic activity, π-complex

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Anode for Electrochemical Ozone Generation Electrolyte-Free Water and Effect This Electrode to Decrease COD

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Abstract: Ozone is an environmentally- friendly oxidant that is widely used for industrial applications, such as water disinfection, air purification, and medical use [1]. Ozone that kills microorganisms, decomposes organic molecules, and removes unwanted components including coloration, cyanide, phenols, iron, and manganese .It can be used to disinfect portable water, food, surgical equipment, and sewage[1]. Ozonation was carried out for COD removal of water [2,3,5,7]. Additionally, ozone is safer than many other disinfectants because it decays to oxygen relatively quickly and leaves no harmful residuals. The efficiency for the oxygen → ozone conversion process ($O_2 + O^\circ \rightarrow O_3$) taking place during silent electric discharge (corona process) depends on several factors: oxygen source (O_2 or air); gas temperature and presence of impurities in the gaseous phase. The efficiency presented by most of the commercially available corona devices, using air as the O_2 source, is 10.4 – 2.0 wt% and requires an "apparent" energy demand (where costs concerning gas refrigeration and heat exchange are not considered) of 114–28 Wh/g. Considering that nitrogen is not an inert gas inside the corona device, this experimental approach using air presents the environmental inconvenience of releasing strong pollutants such as NOx compounds and HNO_3 into the atmosphere. Another commercially available technology for ozone generation is based on electrochemistry (water electrolysis: $3H_2O \rightarrow O_3 + 6H^+ + 6e^-$) [3] . This approach can be achieved by suitable choice of the anode material to have a high over potential 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-PbO_2, Pt, Pt composites, boron-doped diamond, TiO_2 thin films on Si/TiO_x/Pt substrate, and Ti/Ni-Sb-SnO_2 catalysts are among the materials that have been used for EOP.[1-5] In this work, a high-performance porous titanium oxide electrode (Ti/TiO_2/Ni-Sb-SnO_2) has been developed for electrochemical production of ozone .The Ti/TiO_2 electrode was prepared using anodizing method at high voltage for forming a layer of porous TiO_2 on the

surface of Ti mesh, then followed by depositing a layer of Ni-Sb-SnO_2 under deep eutectic solvent on the Ti/TiO_2 surface. The deep eutectic solvent was used for electrodepositing, because its great effect on electrode performance. Ozone was electro generated from tap water on Ti/TiO_2/ Ni-Sb-SnO_2 electrodes at different operating conditions. Higher efficiency of O_3 generation was obtained at 3 V in tap water (Fig. 1a).other electrode only with acidic electrolyte exponent to ozone generation but These electrodes were used in electrochemical ozone production (EOP) carried out during the electrolysis of electrolyte-free water in order to obtain an environmentally friendly technology for water treatment . Figure1b show the influence of COD removal as functions of the ozonation time.

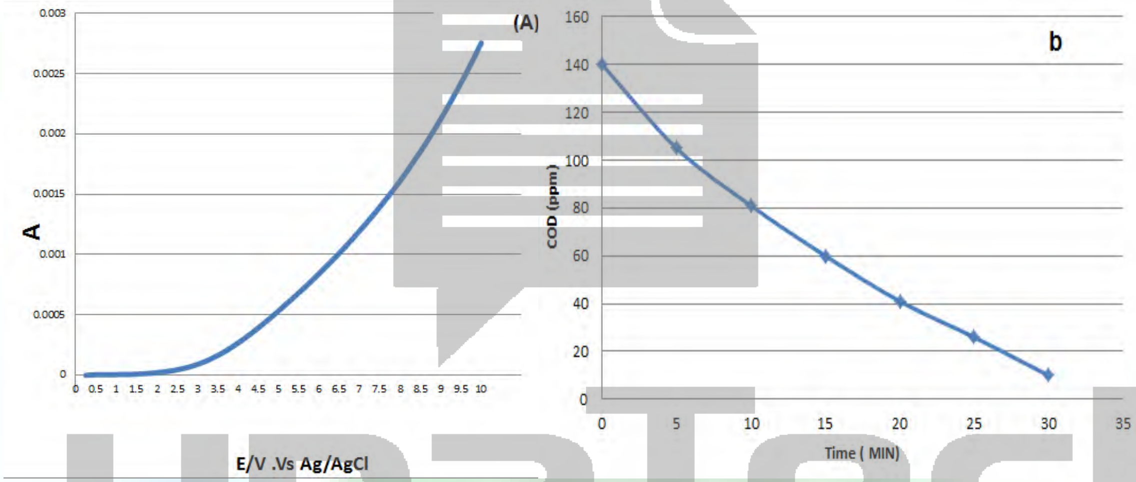

Fig. 1: (a) Anodic linear sweeps at a scan rate of 50 mV/ s in tap water at 25°C E (V) vs. Ag/AgCl/KCl (sat.), and (b)effect of ozone to decrease of COD

References

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In-situ Synthesis of Ag Nanoparticles for High Efficient Reduction of Methylene Blue

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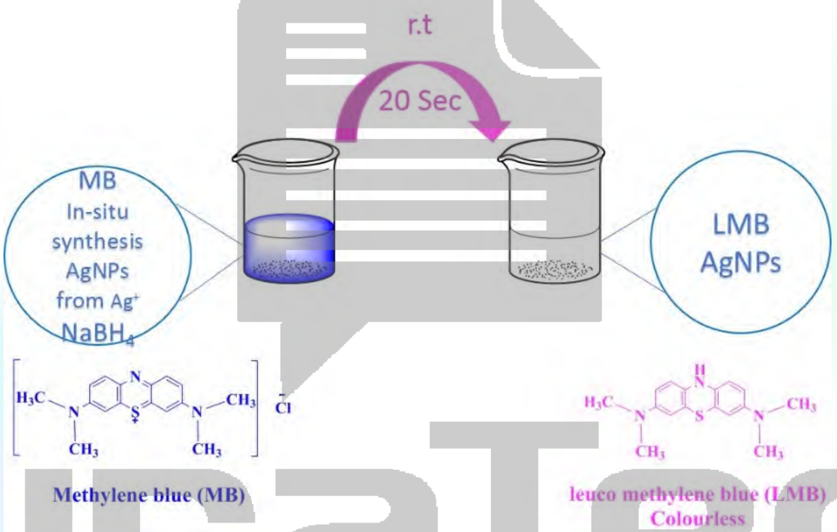
Graphical Abstract



Abstract: Organic dyes in wastewater have become a critical problem due to their nonbiodegradable nature and high toxicity and may have negative effects on human and animal health. For example, the methylene blue (MB), one of the most commonly used organic dyes, can interfere with the photosynthesis and oxygen exchange of aquatic organisms. Thus far, different methods have been developed to address this issue and remove methylene blue from the waste water like adsorption, oxidation, reduction, membrane filtration, and photocatalytic degradation. Among the aforesaid methods, the nanocatalytic reduction of MB into its reduced form, i.e. leucomethylene blue, is more desirable because it has been reported to have many applications in different industrial areas.[1] Herein, we report a rapid, facile, room temperature and one step synthesis for the water soluble Ag nanoparticles (AgNPs) and simultaneous fast and efficient catalytic reduction of MB. In this study, the reduction of MB by sodium borohydride ($NaBH_4$) in the presence of in situ synthesized AgNPs as a homogeneous catalyst at 25°C was conducted and its catalytic activity towards the reduction of MB was studied. The controlled reduction reaction was carried out in which 200 μL of freshly prepared 0.3 M $NaBH_4$ as a reducing agent was added

into 3 mL (10 mg/L) MB solution followed by the addition of 10 μL of 7.5 mM AgNO3 solution as a catalyst. As soon as Ag^+ was added, AgNPs were synthesized in situ in the solution due to the presence of $NaBH_4$ and played role of nanocatalyst, the color of MB solution changed from blue to colorless less than 30 sec. To obtain spectral data and measurement of reduction of MB, UV–Vis absorption spectrophotometer equipped with a diode-array detector was used. The removal efficiency of MB without the catalysts was low, reached about 5% (for MB and $NaBH_4$) within 30min. In the presence of the AgNPs, the MB removal was greatly improved and occurred quickly at the first 20 s and the removal efficiency of 95% obtained. Therefore, the results showed in situ synthesis of AgNPs is a very efficient homogeneous nanocatalyst for the reduction of MB.

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Effective Adsorption of Malachite green oxalate on Modified Layered Double Hydroxide

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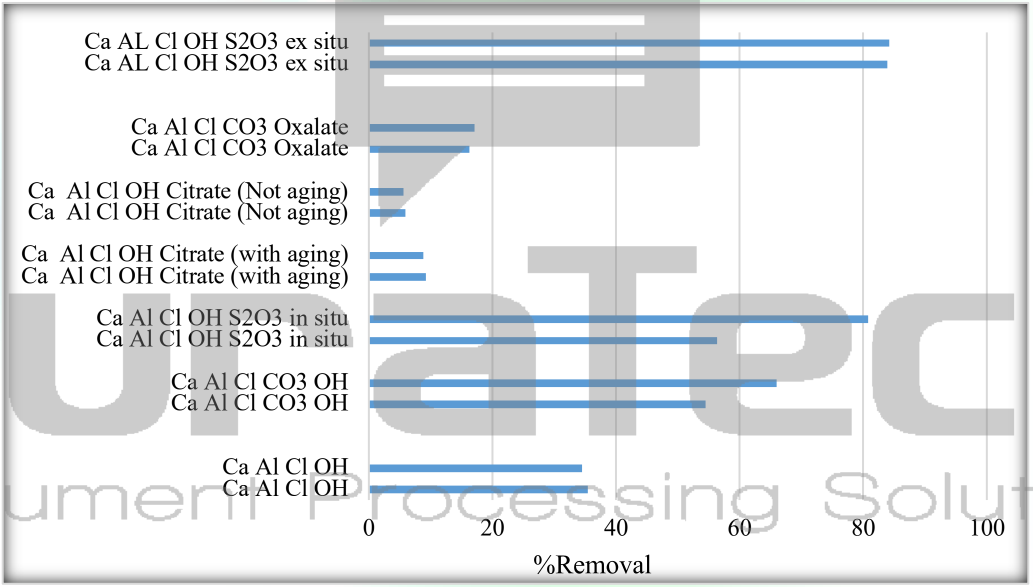
Graphical Abstract



Abstract: Humans are exposed to a variety of environmental pollutants. Cationic triarylmethane dyes such as malachite green are aromatic xenobiotic compounds that causing environmental pollution. Malachite green has been traditionally used as a parasiticide and fungicide in aquaculture and other industries. These compounds are also used as additives in food industries. However, their accumulation in the fish tissues and their carcinogenetic properties, have caused these compounds to be banned from use in the fish food aquaculture in most countries. Also,

regarding this substance, the presence of nitrogen in its structure poses a major threat to the aquatic environment and human health. Therefore, research on the elimination and destruction of this compound in the environment is important. Double layer hydroxides (LDH) are 2D materials that have received attention in adsorption processes due to their easy synthesis, low cost, high surface area, and high adsorption capacity. Theoretically, there is no limit to the type of cations and interlayer anions, which causes a great deal of structural diversity in the LDH family. In the present study, to achieve cost-effective adsorption with the highest removal efficiency, a variety of interlayer anions were examined. Finally, thiosulfate-modified LDH with a removal efficiency of about 90% was used to remove malachite green from the aqueous solution with reproducible results. Identification of the adsorbent was done with some instrumental techniques and optimal parameters in the adsorption process were investigated.

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Synthesis of Arylbenzimidazoles Catalysed by Cu(II) Complex Anchored on The Surface of Graphene Oxide

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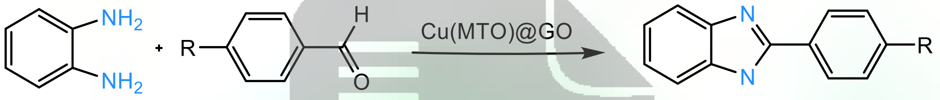
Graphical Abstract



Abstract: Transition metal complexes are one of the most useful and powerful catalysts for industrial processes. However, the practical applications of homogeneous metal complexes are hampered by their high costs with problems of separating from the reaction mixtures [1]. Therefore, designing heterogenized metal complex catalysts is of great interest for economic and environmental reasons in recent years. By being immobilized on insoluble solid materials, the high cost and toxic metal complex catalysts can be easily recovered from the reaction mixtures and ready for reuse [2]. Graphene oxide(GO) -based materials1 are intensively gaining popularity among researchers as novel and promising materials for energy, catalysis and environmental applications [3]. Graphene oxide also has its own advantages compared with graphene. For example, graphene oxide is heavily oxygenated and has hydroxyl and epoxide groups on its basal planes as well as carbonyl and carboxyl groups located at the sheet edges [4]. Recently, graphene oxide with interesting two-dimensional structures and unique properties have emerged as ideal supports for a variety of catalytic species. Besides the availability of surface functionalization, their two-dimensional structures not only allow excellent dispersion of the catalytic species but also facilitate mass transfer in the reaction processes. Herein, we developed an in situ strategy of synthesis and immobilization of a copper complex onto GO support. It was found that the immobilized copper complex with a designed tetrahedral chelate structure not only showed superior catalytic activity for the preparation of arylbenzimidazoles but also exhibited outstanding stability even after intensive reuse, which displays its potential for practical applications.

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GO-Mo-Ni-Layered Double Hydroxide Decorated Amino-Functionalized Zirconium Terephthalate Metal-organic Framework for Extraction of Chlorobenzenes from Solid and Liquid Samples

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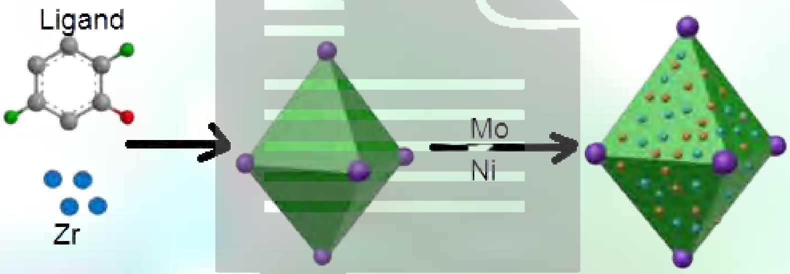
Graphical Abstract



Abstract: Porous materials today include a wide range of compounds that can have a crystalline or amorphous structure, a natural or synthetic base, and an inorganic or organic origin. Until a few decades ago, zeolites and carbon-based materials were considered to be the most important porous inorganic and organic solids. Metal-Organic Frameworks as Porous Mineral-Organic Hybrid Compounds by combining the properties of these two categories have been able to provide further advantages provide. Although all of these compounds are considered to be porous solids, MOFs are different from zeolites in many respects. Structural diversity in MOFs is very high due to the possibility of selecting different components and their ability to operate. However, aluminosilicate zeolites are limited to 4-sided oxide structures. In this study, a new efficient adsorbent of graphene oxide (GO)@Mo-Ni-layered double hydroxides@metal-organic framework (GO@Mo-Ni-LDH@UiO-66-NH2) was synthesized and used for extraction of Chlorobenzens from solid and aqueous samples prior to their determination by GC-MS. The adsorbent was characterized by Fourier Transform Infrared Spectroscopy (FT-IR), Scanning Electron Microscopy (SEM), Energy

Dispersive X-Ray (EDX), X-ray Diffraction (XRD), and Brunauer-Emmett-Teller (BET) analyses. The impact of various parameters affecting the GO-Mo-Ni-LDH@UiO-66-NH_2 process were studied. The main factors such as pH of the aqueous phase, extraction time, amount of adsorbent, type and volume of eluent solvent, desorption time, and sample volume were optimized with a design of experiment technique . The maximum extraction recovery was obtained at an optimized pH 8.0 and extraction time 20.0 min. The adsorption process was fitted by the Langmuir model with a maximum adsorption capacity of 735.12 mg/g. The calibration curve was linear with correlation coefficients ranging from 0.9981–0.9996 for a concentration range of 0.5–100 ng/ml. Under optimum conditions, the limits of detection and quantification ranged from 0.010–0.156 ng/m1 and 0.194–2.30 ng/m1, respectively. Recoveries ranged from 89.6–104.1% with relative standard deviation of less than 1.2%, Furthermore, the GO@Mo-Ni-LDH@UiO-66-NH_2 composite showed high efficiency for the removal of the Chlorobenzenes from environmental Soil and water samples.

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Computational Study of Carbon Dioxide and Carbon Monoxide Conversion to Methanol by Copper Oxide Nanocatalyst from The Environment

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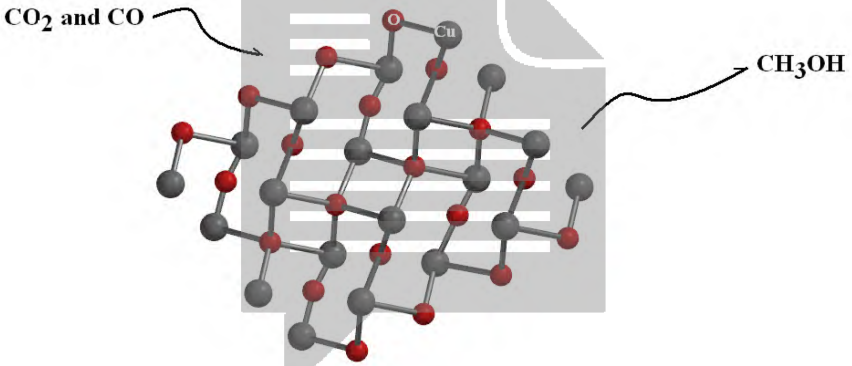
Graphical Abstract



Abstract: One of the important pollutants is carbon monoxide and carbon dioxide that is caused by combustion from different parts of industrial environments, transportation, and so on, which are always the removal and conversion of these two pollutants from the environment is one of the most important environmental issues. In this study, is evaluated and calculated the removal and conversion of these two pollutants at the production site by copper oxide nanocatalyst. All side reactions and by-products of the simulation and their structural and thermosynthetic properties were performed by DFT computational method based on B3LYP/6-31G. Computational parameters show that copper oxide nanocatalysts with monoclonal structure can be used to produce methanol at suitable temperature conditions in gaseous medium.

Keywords: Carbon Dioxide, Carbon Monoxide, Methanol, Formaldehyde, Copper Oxide Nanocatalyst, DFT Computational Method.

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Polyoxometalate-Based Aminofunctionalized Graphene Oxide Catalyst and Its Catalytic Activity for Synthesis of Arylbenzimidazoles

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Graphical Abstract

Abstract: Polyoxometalates (POMs) are a large family of bulky clusters of transition metal oxide anions with structural diversity, showing many applications in catalysis, electronics, optics, medicine, biology, *etc* [1]. Numerous organic transformations can be catalyzed by POMs due to their controllable redox and acidic properties [2]. Polyoxometalates was immobilized on variety heterogeneous supports. Among graphene oxide containing high surface area and reactive morphologies have been studied as effective support for organic reactions [3]. Polyoxometalate (POM)-based graphene oxide prepared with Linqvist type structure have proven to be highly efficient heterogeneous catalysts for the preparation of arylbenzimidazoles, presenting advantages of convenient recovery, steady reuse, simple preparation, and flexible composition. The prepared catalyst was characterized by FT-IR, UV-Vis, SEM, TEM and ICP techniques. The catalytic performances of the hybrid materials were further systematically investigated under various reaction conditions. heterogeneous catalyst can be recycled effectively and reused six cycles with little loss in activity. In addition, the results from hot filtration demonstrated that the catalytic activity mostly resulted from the heterogeneous catalytic.

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A Green Approach for The Electrochemical Dimerization of Edaravone

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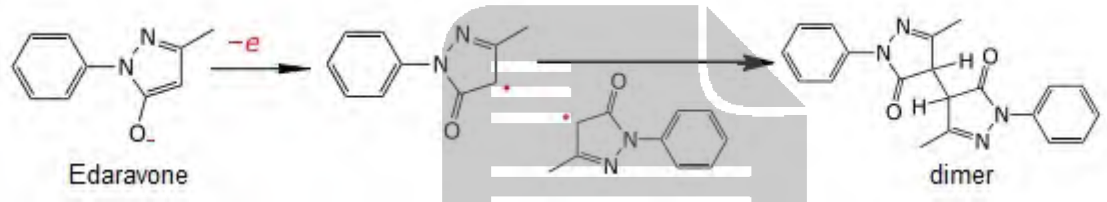
Graphical Abstract



Abstract: Edaravone is a free radical scavenger and neuroprotective agent used for the treatment of acute ischemic stroke and Amyotrophic Lateral Sclerosis (ALS) [1]. Edaravone and its derivatives are also renowned for their antitumor and hypoglycemic activities. Edaravone has attracted the attention of many chemists due to its antioxidant property and free radical scavenging activity [2]. In this work, a green electrochemical method for the synthesis of new dimer of edaravone is described. The electrochemical behavior of edaravone has been investigated in detailed at different pHs regions by cyclic voltammetry and coulometry. Cyclic voltammograms of a edaravone shows an anodic peak, which correspond to the transformation of edaravone to corresponding radical, through an irreversible one electron process. This could be considered as a criterion for the instability and reactivity of radical that is produced at the surface of electrode [3]. The electrochemical synthesis has been successfully performed in an undivided cell using graphite electrode without toxic reagents and solvents using an environmentally friendly method.

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A Heterogeneous Catalyst for Synthesis of Arylbenzothiazoles from Aldehydes

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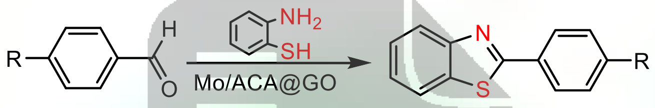
Graphical Abstract



Abstract: Benzannulated heterocycles such as benzothiazoles are very important intermediates in organic reactions [1]. Several methods have been developed for the preparation of these heterocycles including the condensation of aldehydes [2], amides [3], or carboxylic acid derivatives [4] with o-amino thiophenols. The development of efficient and environmentally benign chemical processes or methodologies for widely used heterogeneous recyclable catalyst under solvent-free conditions are one of the major challenges for chemists in organic synthesis. Herein, we wish to report a polyoxometalate- modified graphene oxide hybrid heterogeneous catalysts were synthesized by the reaction of $MoO_2(acac)_2$ with graphene oxide functionalized by grafting procedures of (3-chloropropyl) trimethoxysilane and aminopolycarboxylic acid, respectively. The as-synthesized catalysts were effective in the catalytic in the preparation arylbenzothiazoles. Moreover, the reusability of the catalyst was excellent and the leaching of heterogeneous catalyst was dramatically suppressed. High yields, short reaction times, eco-friendly conditions, simplicity of the procedure, reusability of the catalyst and broad substrate scope are the merits of this protocol.

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Synthesis, Characterization, Crystal Structure and Antibacterial Activity of A Novel Cu(II) Schiff Bass Complex and Using Its Related Nanoparticles to Synthesis of Pyrano[4,3-d]thiazolo[3,2-a]pyrimidine Derivatives

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Abstract: A novel Cu2(L)2Cl4 complex (L= N-(3,4-dimethylphenyl)-pyridine ylmethyleneamine) has been synthesized by two methods. The first method involved the preparation of a single crystal to determine the structure of the complex and Cu2(L)2Cl4 nanoparticles were prepared by the second method. Single crystal X-ray diffraction, NMR, FT-IR, UV–Vis and elemental analysis have been used to characterize the single crystal of the complex(1) and XRD, scanning electron microscopy (SEM), transmission electron microscopy (TEM) and the corresponding particle size distribution histogram has been used to confirm the structure of Cu2(L)2Cl4 nanoparticles(2). The catalytic performance of the Cu2(L)2Cl4 complex prepared has then been assessed in the synthesis of pyrano[4,3-d]thiazolo[3,2-a]pyrimidines derivatives under solvent free conditions in high yields. In addition, all the synthesized compounds were evaluated for their antibacterial activity against Staphylococcus aureus Gram-positive bacteria and Escherichia coli Gram-negative bacteria.

The Environmental Fate and Movement of Organic Solvents in Water, Soil, and Air

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Abstract: Organic solvents are released into the environment by air emissions, industrial and waste-treatment effluents, accidental spillages, leaking tanks, and the land disposal of sol-vent-containing wastes. For example, the polar liquid acetone is used as a solvent and as an intermediate in chemical production. ATSDR1 estimated that about 82 million kg of acetone was released into the atmosphere from manufacturing and processing facilities in the U.S. in 1990. About 582,000 kg of acetone was discharged to water bodies from the same type of facilities in the U.S. ATSDR2 estimated that in 1988 about 48,100 kg of tetrachloroethylene was released to land by manufacturing facilities in the U.S.

Once released, there are numerous physical and chemical mechanisms that will con¬trol how a solvent will move in the environment. As solvents are released into the environ¬ment, they may partition into air, water, and soil phases. While in these phases, solvents may be chemically transformed into other compounds that are less problematic to the envi¬ronment. Understanding how organic solvents partition and behave in the environment has led to better management approaches to solvents and solvent-containing wastes. There are many published reference books written about the environmental fate of organic chemicals in air, water, and soil.3'7 The purpose of this section is to summarize the environmental fate of six groups of solvents (Table 17.1.1) in air, water, and soil. A knowledge of the likely pathways for the environmental fate of organic solvents can serve as the technical basis for the management of solvents and solvent-containing wastes.

Recovery of Uranium from Radioactive Effluents Using Activated Carbon Functionalized with 2-Aminobenzoic Acid

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Abstract: The purpose of this study was modification of activated carbon (AC) to prepare a new selective sorbent for removal of uranium ion. The modification was performed by introducing carboxyl groups onto AC using APS in sulfuric acid solution followed by functionalization with 2-aminobenzoic acid (ABA) as a selective ligand for U(VI) ion (UO22+) adsorption. The characterization of the synthetized sorbent (AC-ABA) was carried out by several methods including potentiometry, scanning electron microscopy, energy dispersive spectroscopy, x-ray diffraction and FT-IR to confirm successful functionalization of the sorbent surface with oxygen and amine groups. The sorption of U(VI) on the unmodified AC and AC-ABA was investigated as a function of contact time, sorbent content, initial uranium concentration, solution pH, and temperature using batch sorption technique. In addition, the effect of various parameters on the U(VI) sorption capacity was optimized by the response surface methodology as a potent experimental design method. The results indicated that sorption of U(VI) under the optimal conditions was significantly improved onto AC-ABA compared to AC. Kinetic studies displayed that the sorption process reached equilibrium after 100 min and followed the pseudo-second-order rate equation. The isothermal data fitted better with the Langmuir model than the Freundlich model. The maximum sorption capacity of AC-ABA for U(VI) was obtained to be 194.2 mg g-1 by the Langmuir model under optimum conditions, which demonstrates the sorption capacity has been improved by the modification process. The thermodynamic parameters (ΔH, ΔS and ΔG) indicated that sorption of uranium onto AC-ABA was an endothermic and spontaneous process. The sorption studies on radioactive effluents of the nuclear fuel plant represented high selectivity of AC-ABA for removal of uranium in the presence of other metal ions, and the selectivity coefficients significantly improved after modification of the sorbent. Application of AC-ABA for treatment of industrial effluents containing heavy and radioactive metal ions show high potential and capability of the proposed method.

Keywords: Waste treatment; Uranium recovery; Nuclear waste; Activated carbon; 2-Aminobenzoic acid

بررسی اثر pH و مقدار جاذب (بر حسب گرم) در حذف باریم از پساب صنعتی با استفاده از نانوجاذب کلسیم آلژینات-اکسید منگنز

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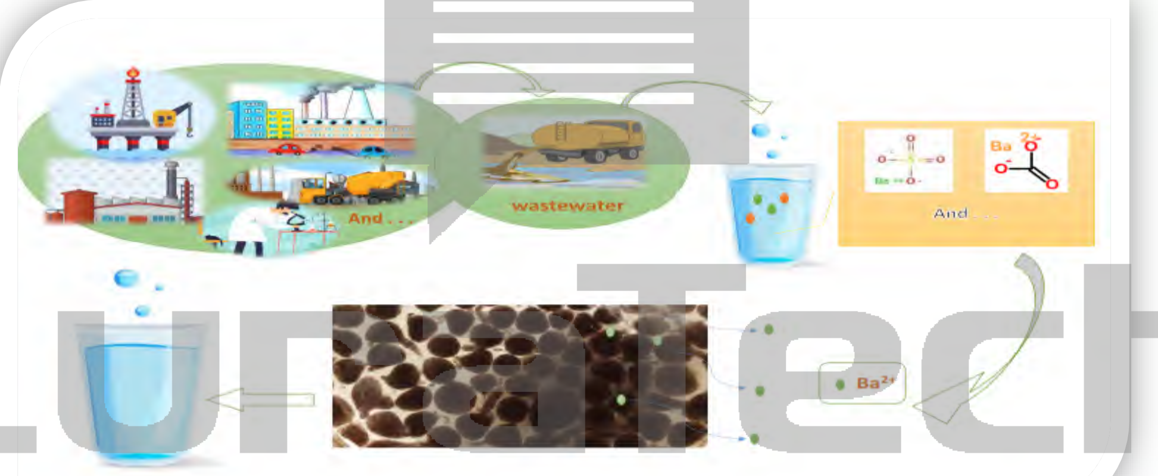
چکیده گرافیکی



چکیده: در این تحقیق جهت حذف باریم از پساب، با نانو جاذب $CaAlg/MnO_2$ انجام شد. میزان جذب یون‌های جذب شده با دستگاه جذب اتمی اندازه گیری شد. در این تحقیق با بررسی اثر pH بر میزان جذب باریم بهینه بدست آمد. در pH =8 حداکثر میزان جذب انجام شد و جاذب باعث جذب بیش از ۸۹ درصد باریم شد. همچنین با بررسی میزان جذب جاذب با مقدار متفاوت جاذب (برحسب گرم)، تقریبا حدود ۸۰ درصد از باریم را جذب کرد. نتایج اولیه این تحقیق نشان داد نانوجاذب سنتز شده به عنوان یک ترکیب طبیعی با کارایی جذب بالا به عنوان نانوجاذب مناسب، می تواند برای حذف باریم از پساب مورد استفاده قرار گیرد.

Improvement of Photocatalytic Degradation of BiOCl Nanostructures by Its Ag-doped for Photodegradation of Environmental Pollutant

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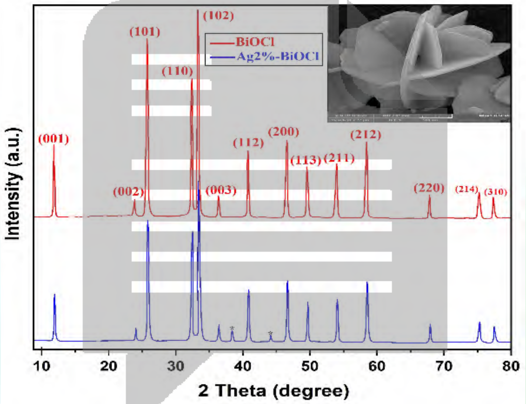
Graphical Abstract



Abstract: In this article, we have tried to improve the photocatalytic performance of bismuth oxychloride (BiOCl) by addition of Ag as dopant to BiOCl nanostructures. The XRD, UV -Vis spectra, and Field emission scanning electron microscopy (FESEM) results confirmed the prepared nanostructures. The effect of some parameters such as pH and the effect of catalyst on both samples in the degradation of reactive black 5 dye (RB5) were also investigated. Degradation of this RB5 at pH = 4 showed its highest percentage and the optimal amount of photocatalyst for the degradation of the contaminant is equal to 5 g L^{-1}.

Investigation of Antibacterial propertise of Hercleum Perscum Extraction PLA-Based Food Packing

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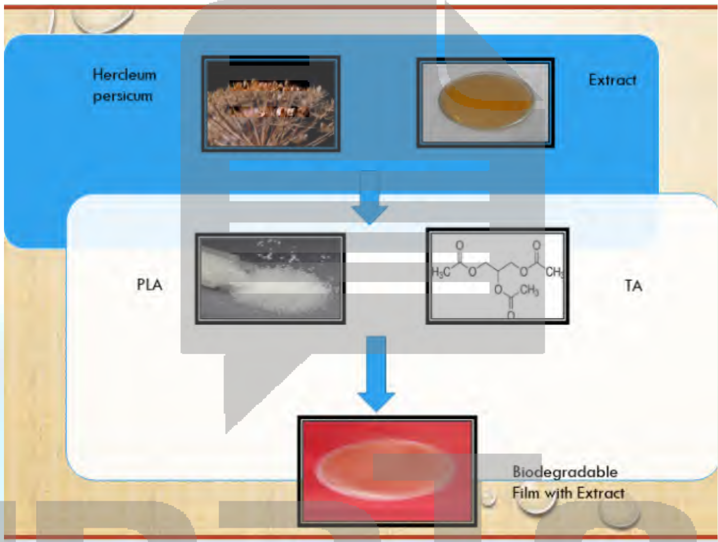
Graphical Abstract



Abstract: In recent years, researchers have paid special attention to biodegradable biopolymer filmsfor food packaging applications due to being biodegradableand environmentally friendly. Here, we investigated the antibacterial activity of triacetine plastisized poly lactic acid(PLA) filmswhen Hercheum persicum extract is added to the polymer mixture. The films are prepared with solvothermal method.

Keyword: Biodegradable , Antibacterial,Film

بررسی قابلیت باگاس نیشکر در حذف رنگ متیلن بلو از پساب

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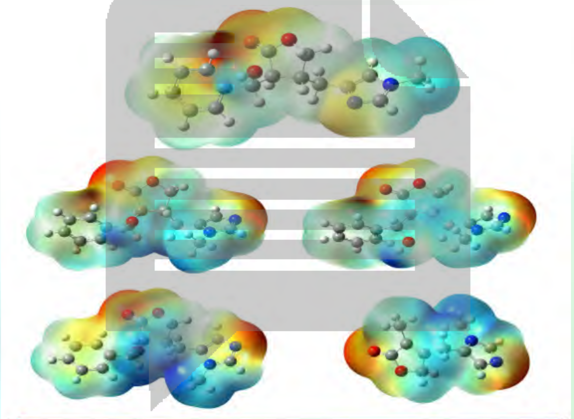
Graphical Abstract



چکیده: در این پژوهش از باگاس نیشکر به عنوان جاذب زیستی، ارازن و دردسترس که همچنین دوستدار محیط زیست می‌باشد برای حذف متیلن بلو از محیط آبی استفاده شد. اثر متغیرهای آزمایشگاهی از جمله اندازه ذرات جاذب، pH محلول، زمان تماس، مقدار غلظت رنگ متیلن‌بلو، سرعت هم‌زدن و مقدار گرم جاذب و همچنین دما بر روی میزان درصد حذف رنگ متیلن‌بلو مورد مطالعه قرار گرفته و بهینه سازی شد. بیشترین کارایی جاذب باگاس برای حذف رنگ متیلن بلو با مقادیر بهینه مش ۱۰۰ برای اندازه ذرات جاذب، pH=۷، مقدار غلظت رنگ ۱ میلی‌گرم بر لیتر، مقدار جاذب ۲۰ میلی‌گرم بر لیتر، زمان تماس ۴۵ دقیقه و سرعت هم‌زدن ۳۰۰ دور بر دقیقه و در دمای ۲۰ درجه سانتی گراد حاصل شد.

کلید واژه: جاذب زیستی، باگاس، رنگ متیلن‌بلو، اسپکتروسکوپی UV-Visb.

Amylodextrin Hydrogel as A Green Sorbent for Pipette Tip Micro Solid Phase Extraction of Triazole Fungicides from Environmental Water Samples

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Abstract: In the present work, a hydrogel was synthesized by combination of hydrophilic acrylic polymers and biodegradable amylodextrin and characterized by Fourier transform-infrared (FT-IR) spectroscopy, Brunauer-Emmett-Teller (BET) surface area, elemental CHN analysis, field emission scanning electron microscopy (FE-SEM) and used as a green sorbent for extraction and preconcentration of triazole fungicides.

Triazole compounds have been globally used for controlling fungal diseases such as rusts, powdery mildews and many leaf-spotting fungi. These compounds have also negative effects on the environment and human health. This research has investigated the determination of triazole fungicides (penconazole,hexaconazole,tebuconazole) in environmental water samples (river water and agricultural wastewater) using pipette tip micro solid phase extraction combined with corona discharge ion mobility spectrometry as a rapid and sensitive detection technique. The effects of important variables on the extraction efficiency were optimized by response surface model (RSM). Under optimum experimental conditions (amount of sorbent: 6 mg, pH of sample solution: 8.0, flow rate of sample solution: 2.0 mL/min, adsorption time: 16.5 min, desorption solvent volume: 1.1 mL, flow rate of desorption solvent: 0.5 mL/min, desorption time: 11.7 min) the technique provided good linearity ($r^2 > 0.995$) over a concentration range of 1.0-1000 ng/mL and repeatability (RSD < 1.7%, n = 5), low limits of detection (0.18-0.20 ng/mL), good preconcentration factors (18.6-19) and high recoveries (93-95%). Finally, the proposed method was applied for quantification of triazoles in environmental water samples.

Keyword: Amylodextrin hydrogel; Environmental water samples; Ion mobility spectrometry; Pipette tip micro solid phase extraction; Triazole fungicides.

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