دانشگاه علم و صنعت ایران
دانشکده شیمی

انجمن شیمی ایران
Iranian Chemical Society

ICC2024
چهارمین کنفرانس کاتالیست
انجمن شیمی ایران

چهارمین
کنفرانس کاتالیست
انجمن شیمی ایران

۹ و ۱۰ اسفند ۱۴۰۲
دانشگاه علم و صنعت ایران
دانشکده شیمی


بسم الله الرحمن الرحیم

سخن دبیر علمی

It is our great pleasure, that the 4th Catalyst Conference was held in Iran University of Science and Technology during November 28 & 29, 2024 (Esfand 9 & 10, 1402), in cooperation with the Iranian Chemical Society. In this two-day conference, the latest scientific and research achievements in various fields of catalysts including homogeneous and heterogeneous catalysts, nanocatalysts, photocatalysts, industrial catalysts, environment, etc. were held according to the themes of the conference. This conference provided an excellent opportunity for professors, researchers, students, chemists, and industrial specialists to present their new findings, research results, and experiences in a friendly scientific community. The primary focus of this significant scientific event in the country was to facilitate discussions and the exchange of current technical knowledge, experiences, challenges, and solutions among experts in the catalyst field. The event aimed to apply the outcomes of scientific research in various areas of catalysts. The scientific committee reviewed and presented the articles submitted by colleagues, students, researchers, and industrialists in lecture and poster formats. In total, 14 lectures and 113 scientific papers were presented in the 4th Catalyst Conference of the Iranian Chemical Society.

Herein, several key scientific and industrial lectures in catalyst-related fields were presented to share the latest experiences and achievements with interested individuals and conference participants, including professors, elites, and experts. In addition to research meetings, there were also industrial gatherings, specialized training workshops, and an exhibition showcasing the capabilities and challenges of related industries and organizations. The conferences aim to encourage and inspire students and graduates in the country. This is an important commitment shared by all universities and scientific associations. Through such events, we hope to instill motivation and hope for a bright future among the attendees. This gathering has the potential to take a strong and effective step towards achieving the goals of Iran's industry and production cycle. With the unity of the academic community, it can lead to the growth and development of both the university and the industry of our beloved country. Finally, I would like to thank all the professors, colleagues, officials of Iran University of Science and Technology, and dear students who helped us organize the 4th catalyst conference of Iran Chemistry Association - Iran University of Science and Technology as best as possible.

With the best regards

Ali Maleki
Professor in Organic Chemistry
The Scientific Secretary of 4th Iranian catalyst Conference

سخن دبیر علمی

بسمه تعالی

با استعانت از خداوند متعال چهارمین کنفرانس کاتالیست با همکاری انجمن شیمی ایران در تاریخ ۹و ۱۰ اسفند ماه ۱۴۰۲ در دانشگاه علم و صنعت ایران برگزار شد. در این کنفرانس دو روزه، آخرین دستاوردهای علمی و پژوهشی در حوزه های مختلف کاتالیست شامل: کاتالیست های همگن و ناهمگن، نانوکاتالیست ها، فوتوکاتالیست ها، کاتالیست های صنعتی، محیط زیست و ... مطابق محورهای کنفرانس برگزار شد. این کنفرانس فرصت خوبی فراهم ساخت تا اساتید دانشگاهی، محققان، پژوهشگران، کارشناسان، دانشجویان و شیمیدانان و متخصصان صنایع در یک اجتماع علمی صمیمی بتوانند تجارب، یافته‌های نوین و نتایج تحقیقات خود را ارائه و با جامعه علمی کشور به اشتراک بگذارند. بحث و تبادل دانش فنی به روز و انتقال تجربیات، بیان چالش ها و ارائه راهکارها و کاربردی نمودن نتایج تحقیقات علمی در زمینه‌های مختلف حوزه کاتالیست اولویت اول این رویداد مهم علمی کشور بود. همچنین مقالات ارسالی همکاران گرامی، دانشجویان عزیز، محققان و صنعتگران از طرف کمیته علمی بررسی و در دو قالب سخنرانی و پوستر ارائه شد. در مجموع در چهارمین کنفرانس کاتالیست انجمن شیمی ایران ۱۴ سخنرانی علمی و ۱۱۳ مقاله علمی ارائه شد.

در این راستا، نشست های صنعتی و کارگاه های آموزشی تخصصی و نمایشگاهی از توانمندی ها، نیاز ها و چالش های صنایع و سازمان های مرتبط به موازات نشست های پژوهشی برگزار شد. همچنین با دعوت از اساتید، نخبگان و صاحب‌نظران چندین سخنرانی کلیدی علمی و صنعتی در زمینه‌های مرتبط با کاتالیست، ارائه شد تا آخرین تجارب و دستاوردهای خود را در اختیار علاقه‌مندان و شرکت‌کنندگان کنفرانس قرار دهند. امید است با برگزاری این‌گونه کنفرانس ها اصل ایجاد انگیزه و امید به آینده روشن برای دانشجویان و دانش‌آموختگان کشور که مورد تعهد تمامی دانشگاه‌های کشور و انجمن های علمی است، تحقق یابد. همچنین این گردهمایی بتواند گامی موثر و استوار در عرصه احقاق اهداف چرخه صنعت و تولیدات کشور با وحدت جامعه دانشگاهی بردارد و به رشد و ترقی دانشگاه و صنعت میهن عزیزمان ایران بینجامد. در آخر از تمام اساتید، همکاران، مسئولین دانشگاه علم و صنعت ایران و دانشجویان عزیزی که در برگزاری هرچه بهتر چهارمین کنفرانس کاتالیست انجمن شیمی ایران- دانشگاه علم و صنعت ایران ما را یاری نمودند، کمال تشکر و قدردانی را دارم.

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حامیان مالی

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Mxenes Photocatalytic Activity for Environmental Remediation Introduction

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Mxenes are a family of two-dimensional (2D) transition metal carbides, nitrides, and carbonitrides. They have attracted significant attention in recent years due to their unique properties, including high conductivity, large surface area, and tunable surface chemistry. Mxenes are typically synthesized by selectively etching the "A" layer from MAX phases, which are layered ternary carbides or nitrides. The resulting 2D structures exhibit a high degree of structural flexibility, allowing for the incorporation of different functional groups and modifications. Mxenes have emerged as a highly promising class of photocatalytic materials for environmental remediation. Their unique properties, including high conductivity, large surface area, and tunable surface chemistry, enable efficient absorption of light across a broad spectrum. The photocatalytic activity of Mxenes has been demonstrated in the degradation of organic pollutants, removal of heavy metals, and bacterial inactivation. These applications highlight the potential of Mxenes in addressing various environmental challenges. However, further research is needed to overcome challenges related to stability, scalability, selectivity, and real-life testing. With continued advancements in the field, Mxenes have the potential to revolutionize environmental remediation and contribute to a cleaner and healthier future.

Keywords: Mxenes, Photocatalytic, Environmental Remediation

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A Review on Bimetallic MOF Structures in Clean Energy Generation

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The increasing global challenges of energy and climate change have led researchers to explore viable solutions, and renewable energy conversion technologies are emerging as sustainable alternatives. Processes like water splitting, nitrogen fixation, and carbon dioxide reduction are crucial in renewable energy systems powered by clean sources like wind, solar, and hydro energy. The efficiency of these chemical reactions heavily relies on catalytic materials attached to electrodes, emphasizing the need for sustainable and efficient catalysts. In the contemporary world, green and sustainable energy conversion technology is pivotal in addressing challenges arising from fossil fuel consumption. Electrochemical processes, such as water splitting, CO_2/CO reduction, and ammonia synthesis, have gained attention for converting renewable energy into high-value chemical compounds. Water splitting, for instance, is a widely studied method for hydrogen production due to its cost-effectiveness, simplicity, scalability, and high efficiency. However, the use of expensive materials like platinum-based electrocatalysts and challenges associated with oxygen evolution reaction (OER) kinetics hinder industrial commercialization. Developing highly active and stable catalysts for optimal OER performance is a significant challenge in energy conversion systems. Metal-organic frameworks (MOFs), especially those derived from bimetallic and heterostructures, show promise as OER catalysts. The porous structure of MOFs offers a large surface area and numerous active sites. The incorporation of carbon-based frameworks enhances electrical conductivity, and the three-dimensional hierarchical porous structure creates additional catalytic sites. Bimetallic and heterostructure catalysts, such as Co/Fe, Fe/Ni, Co/Co_3O_4, NiO/Co_3O_4, Ni_3S_2/Co_3S_4, MoS_2/Mo_2C, and NiMoOx/NiMoS, exhibit superior OER performance due to synergistic effects. However, effective catalyst design remains challenging due to concerns with synthesis reproducibility. Hydrangea-type bimetallic Co/Mo MOF catalysts, utilizing $(Mo\text{-}O_4)^{2-}$ as a molecular binder, are employed for catalyzing the Oxygen Evolution Reaction (OER). The MOF catalysts exhibit an asymmetric Co/Mo_2C surface structure within a nitrogen-doped porous carbon matrix, providing multiple active sites. The molecular binder $(Mo\text{-}O_4)^{2-}$ acts as a connector, contributing to the formation of an effective asymmetric Co/Mo_2C hydrangea-type structure. The resulting catalyst shows promising OER performance with a low overpotential and a Tafel slope, indicating its potential for practical applications. To overcome limitations associated with conventional 3D-MOFs, 2D-MOFs are explored for high-performance OER catalysts. Despite having smaller surface areas, intelligent 2D-MOFs offer advantages like reduced aggregation during pyrolysis, shorter charge/mass transfer routes, and increased active spots on the exposed surface. The synthesis of 2D-MOF-derived catalysts, however, presents challenges due to complexity, time consumption, and non-reproducibility. This review study proposes the utilization of bimetallic Co/Mo hydrangea-type Metal-Organic Frameworks (MOFs) as a pioneering template for highly efficient catalytic structures. The synthesis involves introducing a molecular binder to solvent solutions containing imidazole linkers, resulting in the formation of stereoscopic structures resembling hydrangea flowers. The produced catalysts exhibit distinct nanostructures, demonstrating the potential for high-efficiency Oxygen Evolution Reaction (OER) performance. In conclusion, the research explores the potential of bimetallic Co/Mo MOFs and their derivatives as efficient catalysts for the Oxygen Evolution Reaction. The findings highlight the importance of molecular binders, asymmetric structures, and 2D-MOFs in enhancing catalytic performance for sustainable energy conversion.

Keywords: energy; catalysts; MOF; Nano; Co/Mo

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$CuFe_2O_4$@g-C_3N_4/Carbon dots Based on Waste Biomass as a Promising Photocatalyst for Superior Photocatalytic Oxidation of Toluene to Benzaldehyde under Solar Irradiation

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A prominent mission concerning the area of materials science, particularly, photochemistry would be designing productive photocatalytic system because of the photocatalysis capacity, which acts as an alternate for the purpose of environmental purification and exploiting solar power to compensate energy shortage.

Carbon nanomaterials have emerged and attracted fascinating interests, not only due to their green nature, but also due to their photocatalytic performance. Newly, two-dimensional semiconductors (g-C_3N_4) compared to other materials are in specific value for reasonable reasons of extraordinary features and great potential of being employed in a variety of sectors. More specifically, carbon quantum dots (CQDs) are a novel class of carbon-based nanomaterials with quasi-spherical shape has been proposed as cheap, biocompatible, and non-toxic alternatives to the known toxic materials.

Tailoring of the properties of different materials along with Testing for performance and applications of materials are two vital parts of material science. One of the most common techniques to change the surface properties of nanomaterials for particular applications is surface modification. In this study, according to the low photocatalytic activity of carbon nitride rooted in quick recombination of electrons/holes decision was made to modify the g-C_3N_4. In this regard, nontoxic, economic and convenient magnetic nanocomposite of $CuFe_2O_4$@g-C_3N_4 was fabricated via co-precipitation procedure in the first step. Subsequently, a new carbon dot, which was specifically synthesized for this project added to the fabricated nanocomposite in the next step, then $CuFe_2O_4$@g-C_3N_4/carbon dot was prepared as novel photocatalyst. Additionally, an ingenious prospect has been established to synthesize the carbon dots from soyabean as a biomass waste source by using hydrothermal technique.

The selective photocatalytic oxidation of toluene into benzaldehyde is one of the foremost engaging chemical transformations, which brings a surprisingly perceptible impact on winning different basic natural compounds in both industrial as well as medicinal zones. The genuine worth of the organic reaction procedures gets to be more distinctive when an entirety bundle of green chemistry rules combines into one way to pick up extraordinary efficiencies as opposed to the least inconvenient results on the environment. Due to this objective, using of biomass prepare this work with a green medium as a benign factor, at the same time acting in line with the enhancement of the efficiency of photocatalytic oxidation responses under solar irradiation.

Modification of g-C_3N_4 with $CuFe_2O_4$ and carbon dot reduced its band gap energy from 2.8 to 2.2 eV and made it an ideal candidate for selective photocatalytic oxidation of toluene to corresponding benzaldehyde under 2 h solar irradiation. This work emphasizes the very significant role of materials selection for design and manufacturing processes of new needed products, having the highest attainable quality and performance at the optimum, while meeting the sustainability targets at the same time the due to the rising concerns of environmental aspect. This environmentally friendly approach has demonstrated many advantageous such as process manageable, economical, selectivity, mild reaction conditions, and applying magnetically recyclable photocatalyst under solar irradiation. Moreover, the transformation yield is forecasted to be remarkably increased by employing $CuFe_2O_4$@g-C_3N_4/carbon dot.

Keywords: g-C_3N_4; Carbon dots; Biomass; Photocatalyst; Solar Irradiation

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High performance catalytic CO_2 fixation via a novel mixed linker zirconium MOF under mild condition

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Metal-organic frameworks (MOFs) are a class of porous nanomaterials that consist of organic linkers that coordinate to metal clusters and form infinite crystalline networks with specific topologies and functionalities. The synthesis of multifunctional MOFs can be achieved by various methods including post synthetic functionalization, loading nanomaterials, etc. Using a mixed linker strategy is a novel advanced method in synthesizing functional MOFs, in which different carboxylate linkers incorporates into the MOF structure. This approach enables the introduction of mixed functional groups that are otherwise inaccessible by using a single linker.

In this study, we have designed and synthesized a novel pyrazoledicarboxylic acid linker with electron withdrawing groups and used it as a secondary linker in the synthesis of a mixed linker zirconium-based MOF. The resulting MOF was characterized by various techniques, such as PXRD, FTIR, BET, NMR, etc. and was applied as a heterogeneous catalyst in the cycloaddition reaction of styrene oxide to cyclic carbonate under solvent-free and mild conditions. The catalytic performance of the mixed linker MOF was superior to that of the single linker MOFs, demonstrating the advantages of the mixed linker strategy.

Keywords: Metal-Organic Framework, Mixed Linker, Catalyst, CO_2 fixation

References

Green synthesis of 1H-indazolo[1,2-b] phthalazine-1,6,11(13H)-triones by ZrO(NO3)2.2H2O as a new catalyst and their theoretical studies

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A multicomponent reaction (MCR) is a one-pot reaction that allows easy access to large libraries of organic compounds [1]. This study has revealed some potential leads for possible pharmaceutical applications and further investigations may help in the development of new antioxidative agents for important metabolic functions [2]. In the present work, we have investigated the synthesis of 1*H*-indazolo[1,2-*b*] phthalazine-1,6,11(13*H*)-trione by using $ZrO(NO_3)_2.2H_2O$ as a novel catalyst which have been analyzed by means of the G3MP2 the long-rangecorrected version of the Perdew- Burke-Ernzerhof (PBE) exchange functional (LC-ωPBE),second-order MøllerPlesset perturbation theory (MP2)and hybrid density functional (B3LYP)based methods with the 6-311 + G** basis set on all atoms. The optimized geometries, quantum molecular descriptors, IR spectra data, ^1H NMR and ^{13}C NMR chemical shifts computations, molecular electrostatic potentials (MEPs), the thermodynamic and electronic properties, and NBO analysis have been calculated and carried out [3-4].

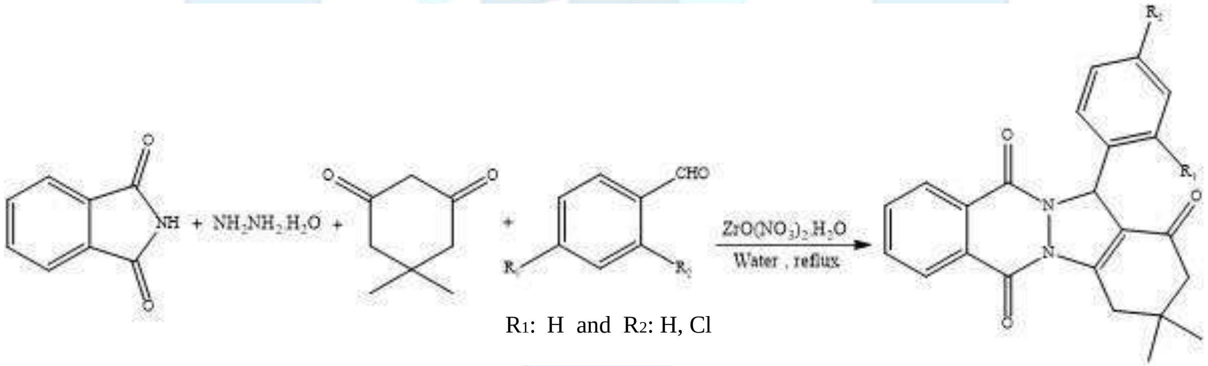

Figure 1. Scheme of the reaction

Keywords: MCR; 1*H*-indazolo[1,2-*b*] phthalazine-1,6,11(13*H*)-trione; $ZrO(NO_3)_2.2H_2O$; B3LYP

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Development of Metal-Organic Frameworks as heterogeneous catalysts: A Review

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Nowadays Metal-organic frameworks and the materials derived from them are getting more attention by reason of their adaptable and versatile tunability and very good catalytic activity.

MOFs are porous materials with metal nodes integrated with organic linkers. In these crystalline materials the secondary building units (SBU) revealed that these materials can be a very good potential for producing networks with sizeable pores and high specific surface areas. This open framework structure makes these materials particularly desirable for diverse catalytic applications.

So far, many investigations have been done which led to numerous articles and new points of view for utilizing these materials as new generation of catalyst in reactions.

The main interest of MOFs (specially ZIFs) lies in the variety of structural adjustment by carefully choosing metal nodes and organic linkers. Supported metal nanoparticles have been led to more attention in recent years since their discovery. As mentioned before out look to catalysis has changed dramatically because of the unique properties of materials like MOFs, ZIFs and COFs owing to these species exhibit compared to those of the bulk.

Among many characteristics of these materials such as their low densities, large surface areas, and high pore volumes and controllable morphology, the development of the porosity, both size and shape in MOFs which is a consequence of the assembly of both metal centers and organic ligands, MOFs demand the use of templates as structural-directing agents, is one of the most important properties of inorganic porous materials.

All these properties, and with the great structural variability of these materials, make Metal-Organic Frameworks highly adaptable, with physico-chemical properties adapted for a specific application.

In this review we attempt to emphasis on reduction and oxidation reactions which are playing a crucial role in industries.

And for this reason, this novel issue needs to be reviewed to be an enlighten for the further and more efforts.

Keywords: Heterogenous catalyst; MOFs; oxidation; reduction

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Preparation, post-synthetic modification, characterization and investigation of the catalytic properties of the Mg/Al-layered double hydroxide

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Epoxides are highly useful intermediates in the production of many chemicals, pharmaceuticals, perfumes, and polymers. In view of the continuing demand for the epoxides, it is imperative to develop greener and sustainable reactions protocols. To address these challenges, highly active, selective and efficient heterogeneous catalysts have been designed. Epoxidation is the chemical reaction, which converts the carbon-carbon double bond into epoxides, using a variety of reagents. Layered double hydroxides (LDHs) are a large family of two-dimensional (2D) anionic clay materials made up of positively charged brucite-like layers with an interlayer region containing charge compensating anions and solvation molecules, which can be represented by the general formula $[M_{1-x}^{II} M_{x}^{III}(OH)_2]^{x+}[A_{x/n}]^{n-}.mH_2O$. The LDH layers incorporate divalent M^{II} (e.g., Mg^{II}, Fe^{II}, Co^{II}, Cu^{II}, Ni^{II}, or Zn^{II}) and trivalent M^{III} metal cations (e.g., Al^{III}, Cr^{III}, Ga^{III}, In^{III}, Mn^{III} or Fe^{III}), forming positively charged layers. A^{n-} are mainly inorganic or organic anions (e.g., CO_3^{2-}, Cl^-, SO_4^{2-}, RCO^{2-}), where x is the molar ratio of M^{II}/M^{III} and generally in the range of 0.20-0.33, which occupy the space between the layers compensating for the positive charge and inducing stability in the overall structure. Despite the unique intrinsic properties of LDHs, various functionalization strategies have been applied to LDHs that yield even more exciting performance opportunities, offering guides to design novel functional nanomaterials. The heterogeneous catalyst for the epoxidation of alkenes is obtained by post-synthetic modification of LDH. Oxo-vanadium (IV) (VO) complexes as a ubiquitous class of transition metal oxo functionalities have received considerable attention due to their wide range of the applications in various oxidation reactions of organic substrates. The good catalytic performance of oxo-vanadium complex in various oxidation reactions were reported, such as the epoxidation of alkene. In this research, the synthesis and identification of Mg/Al-LDH-V catalyst was studied. The results show that the catalyst can be successfully used for the epoxidation of alkenes.

Keywords: Mg/Al-Layered double hydroxide; Epoxidation of alkenes; Oxo-vanadium complex

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Preparation and Characterization of Mesoporous silica Nanoparticles/Copper Acetate as an Efficient Catalyst for the Oxidative Amidation of Benzylic Alcohols

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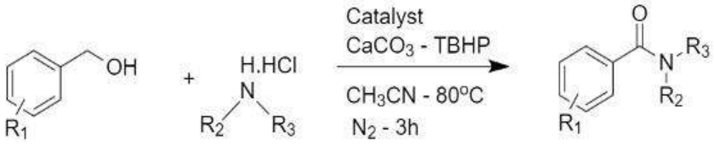
The amide bond is an important linkage in natural products, pharmaceutical compounds, and synthetic polymers. Amide functional groups due to the desirable properties such as high polarity, stability, and many conformational diversities have become one of the most important linkages in organic chemistry. However, the amidation process is a challenge in both the scientific research fields and industrial chemistry. Various methods have been used to synthesize amide, these methods have disadvantages such as difficult reaction conditions and low-level efficiency. For these reasons, researchers are led to create novel and innovative methods. New protocols have been evaluated for the conversion of alcohols to amides via the catalytic tandem oxidation amidation reaction via aldehydes intermediates. Various heterogeneous catalysts have been introduced for this process and one of the most efficient of them is copper salts. To prepare of catalyst for this research, copper (II) acetate was loaded in mesoporous silica nanoparticles (Cu/SiO_2). The conversion of substituted benzyl alcohols to various amides can be efficiently carried out with amine hydrochloride salts via a one-pot direct oxidative amidation reaction using TBHP as a green oxidant in acetonitrile. Notably, the one-pot tandem reaction has several advantages: high activity, facile synthetic method, reusability, and simple work-up. Different derivatives of benzyl alcohols and amine salts were used for this reaction. Also, the solvent, temperature, oxidant, base, and catalyst concentration were optimized. Finally, it was concluded that the reaction was carried out within 3h, in the presence of amine hydrochloride salts (1.0 mmol), benzyl alcohol (1.5 mmol), Cu/SiO_2 (20 mg), acetonitrile (3 ml), calcium carbonate (1.1 equiv), TBHP (4 equiv) at 80 °C under N_2 atmosphere with 70-90% efficiency. Furthermore, this synthesized catalyst can be reused for 5 consecutive runs [1-3].



Scheme 1. Graphical illustration of tandem oxidative amidation of benzylic alcohol.

Keywords: Amidtaion; Oxidation; Benzyl Alcohol; Mesoporous Silica Nanoparticles.

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Conductive NH_2-MIL 101 and MIL 101 MOFs as High-Performance Electrocatalysts for Water Oxidation

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In recent years, metal-organic frameworks (MOFs) have been extensively investigated for diverse heterogeneous catalysis due to their diverse structures and outstanding physical and chemical properties[1]. Currently, most related works focus on employing MOFs as porous substrate materials to fabricate confined nanoparticle or heteroatom-doped electrocatalysts, which must be annealed at high temperatures before application[2], [3]. However, the annealing process usually alters the structure, and considerably reduces the MOF intrinsic active sites [3]. Herein, a simple solvothermal process has been used to synthesize a series of NH_2-MIL 101 and MIL 100 MOFs[1], [3]. The as-prepared MOFs are applied directly as highly efficient oxygen evolution reaction (OER) electrocatalysts with no post-annealing treatment. With the NH_2-MIL 101 and MIL 100 MOFs as the catalyst, the OER current densities of 20 and 50 mA/cm^2 can be achieved at the overpotentials of 290 and 375 mV for NH_2-MIL 101 and 235 and 298 mV for MIL 101. Meanwhile, a small Tafel slope of 84 and 78 mV/dec was obtained, respectively. Moreover, MIL 101 catalyst shows high electrochemical stability in strong basic solution. This work demonstrates that through structural optimizations, MOFs have promising potential as advanced catalysts for electrochemical energy conversion[2].

Keywords: water splitting; electrocatalysis; oxygen evolution reaction; metal-organic frameworks.

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A zirconium-based metal-organic framework (MOF-801) for the efficient adsorption of Cr(VI) from aqueous solutions

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Abstract: Unlike the removal of organic contaminants from aqueous solution, heavy metals are not easily degraded and remain a persistent threat to the environment [1]. The hexavalent chromium Cr(VI) is one of the most dangerous heavy-metal water pollutants according to the World Health Organization (WHO) [2]. In recent years, numerous techniques have been developed for the removal of Cr(VI) from aqueous solution. Among various, adsorption has attracted more attention due to its high efficiency, simplicity, low energy consumption, and recyclability [3]. Metal-organic frameworks (MOFs) have received extensive attention due to their unique crystal structures and excellent properties. MOFs are special coordination polymers formed by the esterification reaction of metal /clusters with organic ligands. Compared with other materials, MOFs have many advantages, including highly crystalline spatial structures, huge specific surface area, and excellent modifiability [4]. In the present study, we have successfully synthesized water-stable MOF-801 and and employed it an effective Cr(VI) removal material from water. The experimental results suggest that MOF-801 has a fast response and high capture capability for Cr(VI). The maximum absorption capacity of MOF-801 at 298 K and pH = 3 was 348 mg/g for Cr(VI) and adsorption equilibrium was reached after 30 min. It was found that Langmuir isotherm is more suitable for describing the adsorption process of Cr(VI) on MOF-801 , indicating that the process is a physically controlled monolayer adsorption. Thermodynamic investigations suggested that the adsorption process is spontaneous ($\Delta G^\circ < 0$), disordered ($\Delta S^\circ > 0$), and endothermic ($\Delta H^\circ > 0$). Besides, MOF-801 displayed an appropriate reusability for the elimination of Cr(VI) ions from their aqueous solutions for 5 successive cycles. In general, MOF-801 has been shown well adsorption properties and reusability, and our finding provide new insights into the development of efficient and reusable adsorbents for Cr(VI) removal.

Keywords: Metal-organic frameworks, Adsorption, Langmuir isotherm.

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Synthesis and application of magnetic nanocomposite hydrogels based on natural gums ($Fe_3O_4@SiO_2$/GO-Hyd) in Synthesis of 2,4,5-triarylimidazoles derivatives.

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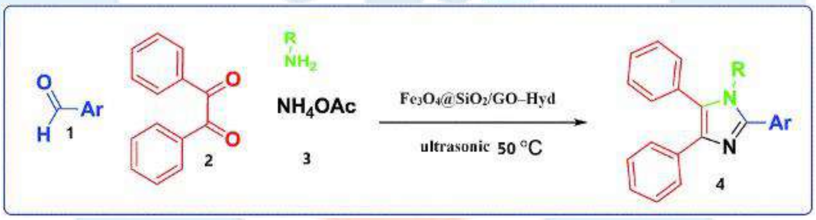
A catalytic methodology for the efficient synthesis of 2,4,5-triarylimidazoles derivatives. The process employs hydrolyzed hydrogels based of Arabic gum ($Fe_3O_4@SiO_2$/GO-Hyd) as an acidic catalyst[1]. This catalyst notably facilitates the activation of carbonyl groups in synthesizing 2,4,5-triarylimidazoles 4, utilizing benzaldehyde 1, benzil 2 and ammonium acetate 3 in an aqueous medium under ultrasonic irradiation[2]. Noteworthy is the catalyst's sustainability, evidenced by its consistent performance over ten usage cycles without noticeable activity loss. The methodological foundation of this protocol is the employment of an environmentally benign, heterogeneous catalyst composed of Fe_3O_4 magnetic particles intricately combined with natural gums as a structural scaffold[3]. The devised bio-based catalyst, characterized by a soft, three-dimensional cross-linked framework, exhibits distinct acidic and basic sites. This feature renders it an efficacious catalyst for the one-pot synthesis of 2,4,5-triarylimidazoles derivatives[4]. The superparamagnetic properties of the nanocomposite enable its facile separation via an external magnet. Moreover, the catalyst maintains its efficacy for at least seven consecutive reaction cycles before a decline in activity is observed[5,6].

FT-IR, TGA, XRD, FESEM, EDX, and VSM methods were used to characterize the produced catalyst. Optimal synthesis conditions were identified as the use of 0.01 g of the catalyst at 50 °C in a water solvent mixture, yielding a maximum output of 2,4,5-triarylimidazoles derivatives of 98% within 15 minutes. The protocol's advantages include its simplicity, short reaction duration, high yield, and the notable reusability and stability of the catalyst.



Synthesis of 2,4,5-triarylimidazoles derivatives in the presence of ($Fe_3O_4@SiO_2$/GO-Hyd)

Keywords: triarylimidazoles derivatives, nanocomposite hydrogels, natural gums.

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Synthesis magnetic nanocomposite hydrogels based on natural gums (GO-Hyd@$ZnFe_3O_4$) in Synthesis of 2,4,5-triarylimidazoles derivatives.

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Keywords: triarylimidazoles derivatives, nanocomposite hydrogels, natural gums.

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A review of enzyme production from agricultural waste: a case study of pectinase

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Every year, millions of tons of rice, wheat, pulses, oilseeds and sugarcane are produced all over the world. Agricultural practices contribute significantly to various industrial sectors such as food, feed, textiles, etc., but still result in the generation of huge amounts of agricultural waste. These wastes are simply burned or buried to rot, which threatens human health and the environment. Meanwhile, renewable and cheap agricultural residues with abundant carbon (lignin, cellulose, hemicellulose, starch and pectin) and nitrogen reserves can act as an ideal raw material for the cost-effective production of various industrial products. Pectinases are a group of enzymes that destroy pectin materials through depolymerization (hydrolase and lyase) or deesterification (esterase). This enzyme is present in the fruit of plants and causes the fruit to ripen naturally. But for large-scale production, microbial sources, including different species of bacteria, fungi, and yeast, are used. Two methods of solid state fermentation (SSF) and immersion fermentation (SmF) are used to produce pectinase. Fruits and vegetables processing, sugaring of agricultural raw materials, beverage industry, vegetable oil extraction, textile material processing, tea and coffee processing, animal food processing, pulp craft bioleaching and paper recycling are among the applications of this type of enzyme. Several studies have investigated the use of sugar beet pomace as a source of pectin to feed microorganisms and produce pectinase. Citrus peels and pomace from apples, tomatoes, peaches, and potatoes are other sources of pectin that have been studied. In this article, some points of pectinase production process and its application are reviewed.

Keywords: Enzyme, pectinase, agricultural waste, biotechnology

Chemical CO2 Fixation Using Perlite/Activated Carbon Catalyst under Solvent-Free Conditions at Low Pressure of CO2

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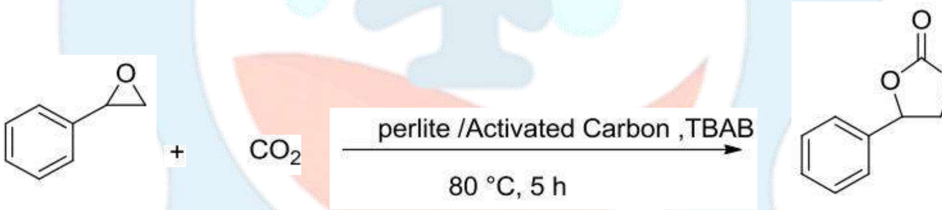
Climate change has caused many problems such as seasonal changes, sea level rise, and endangered ecosystems, and needs effective solutions. One viable approach is to capture and utilize carbon dioxide, with chemical CO2 fixation and its conversion to cyclic carbonate have emerged as one of the best options. In this research, we have introduced Perlite/Activated carbon as an innovative, cost-effective, and environmentally friendly catalyst with multiple active sites. It acts as an efficient catalyst for the synthesis of cyclic carbonate under very mild conditions, including low CO2 pressure and solvent-free conditions, thereby making it both practical and eco-friendly The catalyst and final product were characterized by using NMR, SEM-EDS, XRD, XRF, and FTIR.

Keywords: CO2 Fixation; Perlite/Activated Carbon; Solvent-Free; Low Pressure of CO2



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The synthesis of magnetic Fe_3O_4@MOF composite with high capacity towards drug delivery

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A magnetic MOF composite was successfully synthesized by a sol-gel method. The Fe_3O_4@chitosan core was coated by a shell of nano-ZIF-8 in methanol for high yield, and Fe_3O_4@chitosan@ZIF-8 core-shell nanostructures were obtained successfully that could be used to prevent premature release of loaded drug at physiological environment. Samples were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and vibrating-sample magnetometer (VSM) analysis. The exploration of metal-organic frameworks (MOFs) with good biocompatibility and physiological stability as carrier platforms for biomedical applications is of great importance but remains challenging such as reaching to cancerous tumours [1]. Herein, we modified a zeolitic imidazolate framework (ZIF) nanocrystal by Fe_3O_4 magnetic compound. The magnetic property can be used as an effective agent for drug delivery systems because its capability in iincreasing the probability of the drug reaching the target. On the other hand, various drugs are used to treat cancer; one of the most widely used is doxorubicin (DOX) [2,3]. In order to check the ability of the prepared composite for the drug delivery process, the loading and release properties of the desired drug were investigated, and the results showed that this composite can be used as an effective compound to carry DOX drug.

Keywords: ZIF-8; Drug delivery; DOX

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Microneedle-Based Eye-Readable Biosensor for Futuristic Point-of-Care Prognosis

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Interstitial fluid (ISF), a stable matrix with unique biomarkers, accessible via the skin, allows precise, in situ, and broad disease diagnosis. Microneedles (MNs) enable a user-friendly, painless sampling process, contributing to effective and primary diagnostic procedures[1]. Herein is a minimally invasive biocompatible MN patch utilizing a swellable polyvinyl alcohol (PVA) and polyvinyl pyrrolidone (PVP) hydrogel. This MN patch enables robust ISF extraction by suppressing macromolecular disturbances and sampling the oxalate target analyte, a potential biomarker for kidney disease[2]. The MN patch also integrates a layer-by-layer eye-readable redox-capable sensor through microfluidic channels. This sensor comprises layers of permeable cotton fiber, agarose, and mixed-color etched Mn-Prussian blue analogues, as well as Fe-Prussian blue analogues (AGH-CP/MnFeCN/FeFeCN). Incorporating MnFeCN/FeFeCN with oxidase-like activity in the display layer initiates a reaction between the Prussian blue analogues and 3,3′,5,5′-tetramethylbenzidine[3]. This reaction results in a color change from green to blue, indicative of the oxalate concentration as a radical scavenger. The sensor demonstrates exceptional performance, with detection limits for oxalate at 0.897 μM and 1.22 % RSD. It boasts a linear range of 3.73-186.5 μM, accurately quantifiable by analyzing sample images using a smartphone. The developed microneedle demonstrates satisfactory stability, while the integrated sensor exhibits high selectivity, sensitivity, reliability, and long-term stability[4]. This minimally invasive sensing system, designed for integration with a fixed smart wristband, opens up new possibilities for precision point-of-care monitoring, particularly in the realm of personal healthcare monitoring[5].

Keywords: Colorimetric sensors; Smartphone determination; Ammonia and Acetone VOCs biomarker; Metal-organic frameworks; Eye-readable point-of-care device

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Solid-State Sensor based on Novel Catalyst for Hyperoxaluria Diagnosis

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Oxalates, naturally occurring compounds found in everyday human diets, are typically excreted through the kidneys. However, genetic factors or consuming high-oxalate foods may cause kidney troubles due to excessive oxalate levels, called hyperoxaluria [1]. Early diagnosis and prompt treatment of hyperoxaluria are crucial to prevent long-term kidney damage. In this regard, analysing low levels of oxalate in body fluids can aid in the early-stage diagnosis of the disease. To enable easy and portable monitoring, a specific detection strategy is required to interact with oxalate and provide a visual indication that can be easily interpreted by users. In this context, Mn-Prussian blue analogues (Mn-PBA), mixed with Fe-Prussian blue analogues(PB) with oxidase-like activity as an effective catalyst are encapsulated in a solid-state cotton fibre platform to interact with oxalate as biomarker and 3,3′,5,5′-tetramethylbenzidine (TMB) as chromogenic agent, resulting in a colour change proportional to the various analyte concentration and the oxalate level can be determined visually [2]. To enable quantification, the colour intensity is correlated with the oxalate concentration, and sample images are analysed using a smartphone [3]. This approach allows for accurate quantification of the analyte, providing a user-friendly and portable means of detection. The developed solid-state sensor exhibits excellent selectivity and stability, making it suitable for health management applications [4]. In summary, the use of solid-state sensors for analysing body fluid samples combined with MN-PBA and PB for colorimetric detection offers a practical and feasible strategy for the early diagnosis of hyperoxaluria. The integration of smartphone signalling and the visual detection of oxalate levels further enhances the effectiveness and advanced nature of this approach. The developed solid-state sensor could hold great promise as a wearable sensor for health management, enabling timely intervention and improved outcomes for individuals with hyperoxaluria [5].

Keywords: Colorimetric sensors; Smartphone determination; Solid-state sensor; Oxidase-like activity; Prussian blue analogues.

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[Et3NH][HSO4] As Ionic Liquid Catalyst For Synthesis Of Tetrahydrobenzo [b]Pyrans in aqueous media

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Abstract

The utility of Ionic Liquids (ILs) as catalyst for the environmentally benign synthesis of heterocyclic cmpounds found important for due to their unique chemical and physical properties. These properties of ILs included low vapor pressure, recyclability, controlled miscibility, high thermal and chemical stability. Thus, ILs are safer alternatives to organic synthesis as they are cheap, easy and safer to use that lead clean reactions at short time. The development of a clean synthetic procedure has become crucial in current research due to increasing environmental concerns. There is great demand for the experienced thoughtful changes with more sustainable processes that avoid the extensive use of toxic and hazardous solvents and reagents, tedious reaction conditions, costly and complicated catalytic systems are demanded in recent years. The synthesis of 2-amino- 5,6,7,8-tetrahydro-7,7-dimethyl-4-(3, 4-substituted phenyl)-5-oxo-4H-chromene-3-carbonitrile or tetrahydrobenzo[b]pyran derivatives were successfully synthesized via one pot multicomponent cyclocondensation reaction of aromatic aldehydes, dimedone and malononitrile utilizing triethylamine hydrogen sulphate [Et3NH][HSO4] as ionic liquid catalyst in aqueous media and microwave irradiation method. The reaction was carried to study the optimization of reaction conditions. It was observed that the reaction was best finished when 20 mol% of [Et3NH] [HSO4] ionic liquid catalyst, in aqueous media and MWI conditions are utilized. The ionic liquid catalyst was recycled for three cycles. Our method represents highly efficient, cheap reusable catalyst and environmentally benign greener protocol for the synthesis of chromene-3-carbonitrile or tetrahydrobenzo[b]pyran derivatives in aqueous media conditions.

Keywords: Tetrahydrobenzo[b]pyran, ionic liquid [Et3NH] [HSO4], microwave irradiation, green protocol

Covalently Anchored Cobalte Complex of Salen-type Ligand onto the Surface of Mesoporous MCM-41

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A general strategy for converting a homogeneous process into a heterogeneous one is to anchor the soluble catalyst onto large surface area inorganic supports .The main advantages of heterogenizing the complexes are the easy separation of the catalyst from the reaction mixture, allowing the possibility to recover and reuse the catalyst, and the possibility of continuous-flow operation. The common problem of this methodology is leaching of the active sites from the solid surface into the solutions, when applied to liquid-phase reactions. However, this can be avoided or minimized by covalently anchoring the active sites onto the inorganic solid supports. As a support, MCM 41 silica have been widely used since the performance of this material in catalysis is directly related to a structure possessing hexagonally packed arrays of one dimensional cylindrical pores[1-3]. This work reports the covalent attachment of new salen-type complex of Co on MCM-41, by the new grafting method using 3-aminopropyltrimethoxy silane and application for epoxidation of alkenes by H_2O_2. Additional information was obtained by powder X-ray diffraction (XRD), BEt, GC, FTIR spectroscopy.

Keywords: Cobalt, epoxidation, MCM-41, Immobilization.

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PLA/Graphene/ZIF8 Nanocomposite for Efficient Photocatalytic Degradation of methamphetamine, and ketamine

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Abstract

Illicit drugs have attracted extensive scientific attention as a class of environmental pollutants due to their frequent occurrence, difficult degradability, and potential danger to humans and aquatic animals. Metal-organic frameworks (MOFs) with a high specific active area and porous nature are one of the best candidates to synthesize through the templating method. Zeolitic imidazolate frameworks (ZIFs, based on imidazole bridging with Zn^{2+} or Co^{2+}) are an attractive sub-family of MOFs that combine the benefits of zeolites and MOFs materials [1,2]. ZIFs have become hot topics among the research society due to their outstanding properties such as excellent chemical and solvent stability compared with most other MOFs [3,4]. In this work, PLA/G/ZIF8 nanocomposites were synthesized and used to degrade methamphetamine and ketamine under sunlight. The prepared nanocomposite of PLA/G/ZIF8 nanocomposite was characterized by FT-IR, SEM, XRD and UV-Vis techniques. Also, the mechanical properties of the nanocomposite were investigated using the stress -strain curve. UV-Vis absorption spectrum at different times were used to evaluate the progress of the reaction. In order to achieve the best photodegradation efficiency, pH, type of photocatalyst, the weight of photocatalysts, and illicit drugs concentration were studied. A central composite statistical design was performed and then a second-order polynomial equation was fit to the experimental data with the aid of response surface methodology. The photodegradation of methamphetamine, and ketamine (5 µg/l) was performed by treatment of wastewater solution (adjusted at pH 7.5) with PLA/G/ZIF8 nanocomposite in the 20min where the reaction temperature was set to 45°C. However, by increase in illicit drugs concentration, the required time for photodegradation, may increase. The synthesized nanocomposite showed a very good efficiency in degradation of methamphetamine, and ketamine, so that under optimal conditions, 100% conversion were observed. In present study, graphite nanosheet, not only construct a template for ZIF-8 polyhedrons but also provide a chance for synergistic promoting adsorption behavior via π-π interactions and electrostatic attractions. The enhanced photocatalytic degradation of PLA/G/ZIF8 nanocomposite can be attributed to the increased optical absorption, effective separation and migration of photogenerated charge carriers as a result of introducing G/ZIF8 into the nanostructure. Based on the identified intermediates, repeated hydroxylation of methamphetamine and ketamine and their fragmentation have been proposed for the degradation pathway. Furthermore, after the degradation process, PLA/G/ZIF8 was recovered and used for the next cycle. The results showed that the nanocomposite can perform ten consecutive cycles without a significant decrease in efficiency. The comparison of photocatalytic activity with other catalysts showed that the nanocomposite synthesized in the present research has a higher efficiency in degradation of methamphetamine, and ketamine. The experimental results revealed coupling photocatalysis with solar irradiation as a clean energy source could be utilized for the degradation of methamphetamine, and ketamine in waste water.

Keywords: ZIF8; Graphene; Solar reactor; Photocatalysis; Polylactic acid.

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Photocatalytic Degradation of Ephedrine and Pseudoephedrine in Clandestine Wastewater Using PBT/TiO_2/ZIF-67 Nano Photocatalyst

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Abstract

Removing chemical waste is a crucial step in safeguarding human health and the environment. A new method for achieving this is through photodegradation, which uses photocatalysts and sunlight as a powerful and cost-effective light source[1]. Ephedrine and pseudoephedrine are often used in illegal drug production and are found in secret labs. As a type of organometallic framework (MOF), zeolitic imidazolate frameworks (ZIFs), which are composed of transition metal cations (M) and imidazole-based ligands (lm), are gaining popularity. [2]. In this study, polybutylene terephthalate was doped with a TiO_2/ZIF-67 nano photocatalyst to break down ephedrine and pseudoephedrine in clandestine wastewater. The nano photocatalyst was fabricated by sol-gel and electrospinning process then it was characterized through FT-IR spectroscopy, SEM-EDX, thermogravimetric (TG) and XRD analyses. In the experimental part, the destruction of ephedrine and pseudoephedrine was studied in photocatalytic degradation on a stainless steel mesh coated with a nanocomposite of polybutylene terephthalate/titanium oxide/ ZIF-67 (PBT/TiO_2/ZIF-67). To achieve the best photodegradation efficiency, sample volume per experiment, pH, ephedrine and pseudoephedrine concentration, temperature, and the percentage of photocatalysts, were studied. PBT/TiO_2/ZIF-67 nanocomposite is a cheap photocatalyst, non-toxic, with a simple preparation method, and could destroy ephedrine and pseudoephedrine with high degradation efficiency. The composites showed higher photocatalytic activity than pure TiO_2 or pure ZIF-67. The results show that the ZIF-67 could be dispersed better in TiO_2 substrate by sol-gel method than by incipient wetness method; the PBT/TiO_2/ZIF-67 nanocomposite prepared by electrospining method had a higher photoactivity performance; moreover, the reaction was dependent on ZIF-67 loading. The efficiency of the photocatalytic process was evaluated with GC-FID analyses. The lifetime experiment for one electrospun leaf showed no significant loss in performance of composite coating over 20 times of photodegradation owing to the high chemical stability of PBT/TiO_2/ZIF-67 nanocomposite. The nanophotocatalysts prepared exhibit superior thermal and mechanical stability and high relative recovery compared to conventional photocatalysts. These properties make them ideal for degrading ephedrine and pseudoephedrine in clandestine wastewater.

Keywords: PBT/TiO_2/ZIF-67; Ephedrine; Pseudoephedrine; Nano-photocatalyst

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Enhancing Photocatalytic Degradation of Rhodamine B (RhB) with Cu-Decorated CdS Nanorods

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This study reports the development of a CdS/Cu nanocomposite photocatalyst with enhanced activity for Rhodamine B (RhB) degradation under visible light. Cu nanoparticles were grown in situ on CdS nanorods, exploiting their surface plasmon resonance and creating a Schottky junction to promote charge separation. Characterization confirmed the formation of well-defined CdS/Cu composites with an average Cu nanoparticle size of ~50 nm. Photocatalytic experiments demonstrated significantly improved RhB degradation compared to pure CdS, achieving complete degradation within 90 minutes for 50 ppm RhB. The enhanced activity is attributed to synergistic effects: SPR promoting light absorption, intimate contact facilitating electron transfer, Schottky junction boosting charge separation, and Cu's higher redox potential generating stronger oxidizing species. This work highlights the potential of CdS/Cu nanocomposites as cost-effective and efficient photocatalysts for wastewater treatment.

Keywords: Photocatalysis; CdS/Cu nanocomposite; Rhodamine B degradation.

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Use of reusable cerium oxide catalyst to prepare 3-aryl-4H-benzo [1,4] thiazin-2-amine compounds

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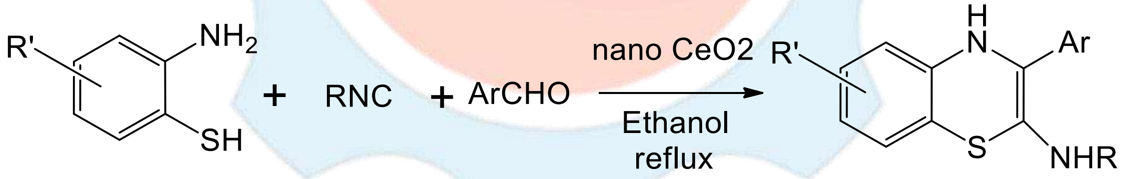
Benzo[1,4]thiazine-2-amine has many biological activities in wide therapeutic fields, including vasodilator, antidiabetic, anticataract, antiarrhythmic, etc. [1-3]. Due to their known biological activities, benzothiazines have many applications in the field of medicine and agriculture [3-6]. Therefore, finding suitable methods for these widely used compounds is of great importance. Various methods have been proposed for the synthesis of these compounds, but most of them have disadvantages and efforts should be made to optimize the methods.

As part of our program aimed at developing new methods for the preparation of new compounds[7], we would like to report one-pot synthesis of 3-aryl-4H-benzo [1,4] thiazin-2-amines via a three-component reaction of an aromatic aldehyde, isocyanide and o-amino thiophenol using nano cerium oxide as a reusable catalyst.

In order to determine the nano size of the nano cerium oxide catalyst, XRD,SEM,TEM methods was used.

This nano catalyst has worked very effectively in the synthesis of these compounds and prepared these compounds with much higher efficiency and in a shorter time than other reported articles.

The reaction products were prepared in moderate to good yields. Moreover, the procedure offers several advantages including high yields, operational simplicity and cleaner reaction which make it a useful and attractive process for the synthesis of these compounds.



Keywords: benzo [1,4] thiazin-2-amine; Aromatic aldehyde; reusable catalyst; cerium oxide

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Application of nickel oxide / aluminum oxide catalyst as an effective and recyclable catalyst in the synthesis of 1,8-dioxohydroxanthenes compounds

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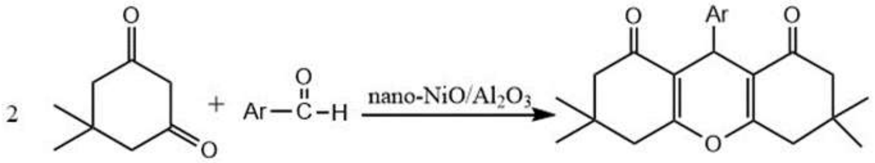
1,8-dioxohydroXanthenes are an important group of biologically active heterocycles and exist in different forms (caffeine, theophylline, theobromine, etc.) in tea, coffee, cocoa, chocolate, etc., which have given them public fame. These compounds are mostly known for their diverse medicinal applications such as cyclic nucleotide phosphodiesterase inhibition, adenosine receptor antagonism, anti-inflammatory, antimicrobial, antioxidant and anti-tumor activities[1-3]. Also, xanthines are a well-known group of alkaloids that are commonly used as bronchodilators and psychological and cardiac stimulants. These compounds are polyaromatic cyclic ethers that have a tetrahydropyran ring attached to aromatic rings and form important groups of oxygenated heterocycles. Various methods have been proposed for the synthesis of these compounds[4-8], but most of them have disadvantages and efforts should be made to optimize the methods In this research, an easy and effective method for the synthesis of 1,8-dioxohydroXanthenes derivatives in the presence of nickel oxide/ aluminum oxide has been presented, which has advantages such as compatibility with the environment, low cost, excellent efficiency and simple work method. Nano nickel oxide/aluminum oxide presented a good performance as the catalyst in synthesizing bis(indolyl)methane and their nano size was identified by XRD,SEM,TEM methods. This reaction was compared with the previously performed reactions and the highest efficiency and the shortest reaction time is in the presence of nano nickel oxide/aluminum oxide catalyst.



Keywords: 1,8-dioxohydroXanthenes; Aromatic aldehyde; recyclable catalyst; nano nickel oxide/aluminum oxide

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Efficient synthesis of bis(indolyl)methane compounds in the presence of nickel oxide/aluminum oxide nanocatalyst as a recyclable catalyst

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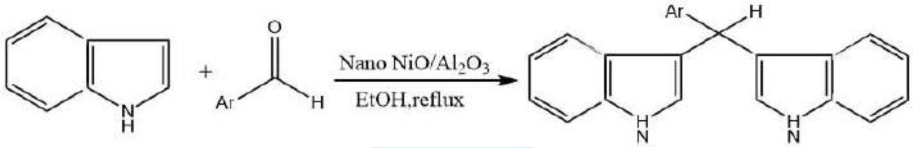
Indoles are one of the first group of antioxidant and anticancer chemical compounds found in food, and scientific experiments have shown that they are very successful in controlling cancer in animals. Indole chemical compounds play their role in preventing cancer through the detoxification of carcinogens. In humans, indoles have shown brilliant results for the prevention of colon cancer and breast cancer and have shown positive effects in the metabolism of estrogen hormone in women. The indole nucleus is present in important pharmaceutical compounds such as sumatriptan, which is used in the treatment of migraine. Various methods are available for the synthesis of indoles[1-3], but they have disadvantages that due to the great importance of these compounds, the effort to invent a more suitable method is still left. In this research, we report the synthesis of bis(indolyl)methane derivatives during the reaction of indole and aromatic aldehyde using nickel oxide/aluminum oxide nanocatalyst as an reusable catalyst. and the following results are concluded:

1.Nano nickel oxide/aluminum oxide presented a good performance as the catalyst in synthesizing bis(indolyl)methane and their nano size was identified by XRD,SEM,TEM methods.
2.The reaction could be investigated and terminated using Thin Layer Chromatography (TLC).
3.The prepared products could be separated easily using filter paper.
4.No lateral products were observed during the reaction.
5.This reaction was compared with the previously performed reactions and the highest efficiency and the shortest reaction time is in the presence of nano nickel oxide/aluminum oxide catalyst.



Keywords: bis (indolyl) methanes;Aromatic aldehyde; recyclable catalyst; nano nickel oxide/aluminum oxide

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Synthesis/Characterization and Application of Fe_2O_3@ZnO Nanocomposite as Photocatalyst to Decontamination of Amoxicillin

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Environmental pollution poses an ongoing challenge for humanity, impeding sustainable development and posing a threat to human health and life. Contaminants of emerging concern (CECs) constitute a category of pollutants resistant to conventional water treatment methods for human consumption, escaping regulation by current environmental laws [1]. Among these CECs, antibiotics have garnered significant attention due to their excessive use in humans, livestock, and aquaculture. Their presence in wastewater, coupled with adverse effects on ecosystems, highlights the need for attention. These drugs enter aquatic environments through diverse sources such as the pharmaceutical industry, hospital effluents, human and animal excretion, improper drug disposal in landfills, and sewage networks, contributing to environmental pollution. Antibiotic residues in aqueous systems, even at low concentrations, can lead to detrimental environmental effects, including antibiotic resistance, disruptions in ecosystems, and potential risks to human health via drinking water and the food chain [2]. Amoxicillin, a widely used antibiotic for human infections, exhibits a significant excretion rate in humans. Reports indicate that over 80% of orally administered amoxicillin is excreted through urine within two hours of ingestion. Current reports show concentrations of amoxicillin in hospital, industrial, and domestic wastewaters ranging from ng/L to mg/L [3]. Various techniques have been employed to eliminate antibiotics from different mediums, including adsorption, advanced oxidation processes, and membrane filtration. Among these, advanced oxidation processes (AOPs) stand out as the most effective for pharmaceutical removal. AOPs utilize hydroxyl radicals to oxidize organic compounds into harmless products and operate efficiently under ambient conditions, harnessing sunlight as an energy source [4]. Photocatalysis, an emerging AOP technique, utilizes nanometer-sized catalysts and light as an energy source to initiate chemical reactions. This study explores the degradation of amoxicillin in water or wastewater samples using the photocatalyst composite Fe_2O_3@ZnO. The synthesized nanocatalyst was characterized through XRD, SEM, TEM, BET, and Zeta-potential analyses. Results demonstrate that Vis/Fe_2O_3@ZnO degraded almost 95% of amoxicillin at room temperature over a 45-minute period, with a first-order kinetics rate constant of 0.0536 min-1. BET analysis indicates that the Fe_2O_3@ZnO photocatalyst possesses nanonet structures with a high specific surface area, enhancing its photocatalytic performance in amoxicillin degradation. The photocatalytic activity of Fe_2O_3@ZnO (95%) surpasses that of pristine Fe_2O_3 (79%) and ZnO (77%).

Keywords: Decontamination; Amoxicillin; Photocatalyst; Fe_2O_3@ZnO Nanocomposite.

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Synthesis of heterstructure photocatalyst Fe_3O_4/g-C_3N_4 and investigation of its photocatalytic behavior in aqueous solutions

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In order to develop degradable technology to correct environmental problems, preparation of an effective hybrid structure photocatalyst for photocatalytic decomposition has been suggested. Binary magnetic nanocomposite Fe_3O_4/g-C_3N_4(F/gCN) was prepared by electrostatic self-assembly method and was identified by XRD, FT-IR, FESEM, VSM and nitrogen adsorption and desorption analysis. The effective factor of pH on photocatalytic performance, the hybrid photocatalyst prepared for degradation of organic pollutant rhodamine B (RhB) was investigated under visible light in aqueous environment. The amount of degradation efficiency by F/gCN nanocomposite at pH= 5,7 and 9 was obtained as 78%, 68% and 64%, respectively. The F/gCN nanocomposite showed superparamagnetic behavior with a saturation magnetization of 20.77emu.g^{-1}, it can actually be separated from the solution and reused. The kinetics of the RhB degradation reaction follows the first order reaction equation and the apparent degradation constants at pH = 5,7 and 9 are estimated to be 0.61, 0.51 and 0.47 min^{-1}, respectively. These results show that the hybrid of iron oxide and graphite carbon nitride is an efficient semiconductor to decompose organic dyes from wastewater.

Keywords: magnetic nanoparticles; graphitic carbon nitride; photocatalytic performance; synetics; rhodamine B

Bioelectrocatalytic effects of a short oligonucleotide sequence on β -Hydroxy Acids and Esters

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Nanoscale materials and their characterizations have opened up new opportunities for the development of cost-effective bioelectrocatalysts due to their exceptional physical and chemical properties [1-4]. Nowadays, proteins, nucleic acids, organelles, whole cells and even intact tissues have all been used as key components in electrode-driven biocatalysis. As biological targets may be present in only trace amounts, electrocatalysis offers a simple and effective method of signal amplification, thereby greatly increasing the sensitivity and on/off signal differential of an electrochemical assay [5-7]. To date, most electrochemical nucleic acid sensors have focused on the detection of hybridization events [8, 9].

In this work, we have focused upon direct electrochemical signals of short double-stranded DNA with salicylic acid (SA) and acetylsalicylic acid (ASA) as will be explained: A short oligonucleotide sequence composed of deoxyguanosine (dG) nucleotides was immobilized on carbonized polyaniline nanofibers (CPANI), and then, hybridized with (dC). The electrocatalytic characteristics of the double-stranded DNA (dG.dC) were investigated by cyclic voltammetry (CV), differential pulse voltammetry (DPV) and electrochemical impedance spectroscopy (EIS) methods. Based on the obtained results, this high surface area modified electrode shows an increase in the DPV current due to the oxidation of guanine. Moreover, the obtained binding constant of these interactions are higher than 10^6 for SA and ASA.

Keywords: Electrochemical nanobiocatalysis, Electrically conducting polymers, Oligonucleotide, Salicylic acid, Aspirin;

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Signal Amplification of Immobilized Genomic DNA on Carbonized Polyaniline Nanofibers

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Bioelectrocatalysis is an important and unique combination of biocatalytic and electrochemically reactions. High specificity and selectivity are the main advantage of electroactive biomaterials and target reactants compared to inorganic materials [1-3]. In the recent years, by connecting deoxyribonucleic acid (DNA) to porous electrodes, it can be exploited high specific biosensors for detecting various biomaterials. For example, polyamines are ubiquitous low molecular weight aliphatic cations, which are involved in a large number of cellular processes including functioning of ion channels, nucleic acid packaging, DNA replication, apoptosis, transcription and translation [4, 5]. Due to their polycationic nature, polyamines are fully protonated under physiological pH and ionic strength conditions. Therefore, these multivalent cations also act as electrostatic bridges between the phosphate charges of DNA, RNA, ATP, phospholipids, or proteins [6].

In this work, we have demonstrated a simple, label free nanobiosensor for studying the electrochemical behavior of genomic DNA (GDNA). Circular dichroism (CD) has been used, to confirm the formation and stability of parallel form of GDNA in the solution using the named oligonucleotide. Bioelectrocatalytic characteristics of the immobilized GDNA has been investigated at the presence of ethidium bromide/polyamines (spermine or spermidine) by different electrochemical techniques. The interaction of GDNA with these two groups of compounds have been investigated. By comparing the values of the binding constant, the mode of interaction of each ligand with GDNA through intercalation or electrostatic binding can be estimated. The results show that the prepared modified electrode has a good correlation coefficient and detection limit for interaction ethidium bromide and GDNA at pH =7.5.

Keywords: Nanobiocatalysis, Carbonized Polyaniline, Ethidium Bromide, GDNA, Polyamines;

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wastewater treatment with chromate nanoparticles as photocatalyst under visible light

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Spinel is a cubic structure with the public formula AB_2O_4, that A and B are cations settled in the tetrahedral and octahedral positions, respectively. therefore, a spinel has 56 atoms in any one cell. The dispensation of ions in A and B sites are subject to the ion equilibrium [1]. Materials and it Nanotechnology is an interdisciplinary knowledge, it is the interdisciplinary, including toxicology, medical, physics, chemistry, biology, mechanics, engineering, and recently environment [2]. in the last decade, environmental pollution has enhancement more and more public worry. for example, wastewater including dyes arriving from paper, textiles, plastic and leather industries is usually high in organic compounds and color [3]. This pollutant agent creates important environmental problems. So, providing effective and efficient method for their removal from wastewater is necessary. Photocatalysis is one of this efficient approach to remove the dyes from wastewater [4]. Among the pollutant agent, we can point to organic dyes from industrial processes and textile as one of the main polluting water sources and create an important environmental crisis. Photocatalysis is considered as one of the important and efficient approaches to dismiss the dyes in wastewater [5]. In this paper a novel and inexpensive route for the preparation of spinel $CoCrMnO_4$ nanoparticles is proposed and Congo red was used as model dye. The obtained nanoparticles were then identified using different analytical techniques such as Fourier transform infrared spectroscopy (FTIR), X-ray powder diffraction (XRD), and field emission scanning electron microscopy (FESEM). The X-ray powder diffraction (XRD) confirmed the formation of cubic spinel phase $CoCrMnO_4$. The photocatalytic activity of $CoCrMnO_4$ nanoparticles were studied by performing the decomposition of Congo red dye under visible light irradiation. The effects of process parameters like, catalyst dosage, initial dye concentration, and visible light irradiation on dye degradation have been investigated.

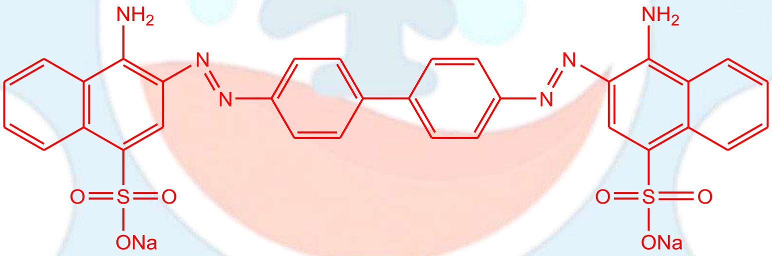

Fig 1. *structure of Congo red*

Keywords: $CoCrMnO_4$ Spinel nanoparticles, Photocatalytic activity, Congo red.

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PVC/$NiAl_2O_3$/AlF_3 nanocomposite: Synthesis and characteristic by Sol-Gel method

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Abstract

Recently, Aluminum Fluoride (nAF) nanoparticles synthesized by the sol-gel method and studied nano-sized morphology of crystals. In other section, the nanocomposite was successfully prepared and characterized by FT-IR, and HRTEM techniques. A solvothermal method has been successfully introduced and applied for nanocatalyst efficiency. Meanwhile, precursor gel preparation and the interaction on the nano-sized area have been studied. This study development exhibited that PVC/$NiAl_2O_3$/AlF_3 (nPNA) nanocomposite as an effective catalyst for the synthesis of some organic derivatives. The results show that the as-prepared nanocomposite is as an efficient catalyst and show that nPNA can be used in next generation some organic reactions and faster produce of various materials.

Keywords: *Morphology; Sol-gel; TEM; Nano Catalytic activity; Nano-Size.*

Palladium Nanoparticles-Decorated Metal-Organic-Framework (UiO-66-COOH) @ 5-Aminotetrazole: Novel Efficient Catalyst in O-Arylation Reactions

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In this research, we prepared highly efficient and reusable catalyst through step-by-step post-synthesis modification of UiO-66-COOH metal-organic framework (MOF) as support with nitrogen-rich as organic ligand in order to synthesis of catalyst named UiO-66-COOH @ 5-aminotetrazole/Pd-NPs [1]. This research is motivated to identify newly synthesized MOF nano-catalyst through metal-organic framework UiO-66-Type with free carboxylic acid as an efficient MOF functionalized 5-aminotetrazole and decoration of palladium - nanoparticles. An efficient catalyst UiO-66-COOH @ 5-aminotetrazole @ Pd-NPs as a heterogeneous catalyst has been applied to O-arylation reactions which have been investigated. The proposed catalyst represented superior catalytic performance for promoting the O-arylation reactions in green aquatic media [2]. The results of productivity catalyst are accomplished in good to excellent yields under mild conditions which is a proof of superior activity heterogeneous catalyst containing Pd-nanoparticles [3,4]. In addition, the suggested catalyst represented excellent reusability with no remarkable loss in activity up 7 sequential runs. In addition, the characterization of the prepared nano-materials were performed using different analyses such as FTIR, XRD, SEM, EDS, TEM, and BET and the results proved the successful synthesize of UiO-66-COOH / Palladium-nanocomposite.

Keywords: nano porous, nano structures, porous metal organic frameworks, O-arylation reaction

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Stabilization of Gold Nanoparticles-Decorated UiO-66-COOH@ 2-Aminopyrimidine: Novel and Efficient Catalyst in C-C Coupling Reactions

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In this research, we prepared a highly efficient and reusable catalyst *via* a step-by-step post-synthesis modification of UiO-66-COOH metal-organic framework (MOF) with nitrogen organic ligand as support for the preparation of UiO-66-COOH @ 2-aminopyrimidine/Au-NPs [1]. This project is motivated to identify newly synthesized MOF nano-catalyst *via* metal-organic frameworks UiO-66-Type with free carboxylic acid as a novel and efficient MOF functionalized 2-aminopyrimidine *via* decoration of Gold-nanoparticles. In order to prepare a highly efficient catalyst UiO-66-COOH @ 2-aminopyrimidine @ Au-NPs as a heterogeneous catalyst for preparation in order to C-C coupling reactions which have been investigated [2,3]. In addition, the characterization of the prepared nano materials were performed using different analyses such as FTIR, XRD, SEM, EDS, TEM, and BET and the results proved the successful synthesize of UiO-66-COOH / Gold-nanocomposite. The proposed catalyst represented superior catalytic performance for promoting the C-C coupling reactions in green aquatic media. The results of productivity catalyst are accomplished in excellent yields under mild conditions which is a proof of superior activity heterogeneous catalyst containing Au-nanoparticles. In addition, the suggested catalyst represented excellent reusability with no remarkable loss in activity up 6 sequential runs.

Keywords: nano porous, nano structures, porous metal organic frameworks, C-C Coupling Reaction, Gold nanoparticles

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Lanthanide Coordination Polymers as Heterogeneous Lewis Acid Catalysts for Glycerol Acetalization

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Coordination polymers containing lanthanide ions (LnCPs) have received relatively less attention compared to d-block metal coordination polymers, despite their potential for remarkable luminescence, catalytic activity, and magnetic properties [1,2]. LnCPs have shown promise as Lewis acid catalysts for various chemical transformations. Lewis acids are electron acceptors that can facilitate chemical reactions by accepting electron pairs from other molecules [3]. The use of lanthanide ions as Lewis acid catalysts is of particular interest, and researchers have been exploring their potential in this area [4].

$[Er_2(bpndc)_3(DMF)_2]$ (**1**) and $[Yb_2(bpndc)_3(DMF)_2]$ (**2**) were synthesized by combining Benzophenone-4,4'-dicarboxylate (bpndc2-) linker, Erbium nitrate hexahydrate, Ytterbium nitrate hexahydrate, respectively, using a facile solvothermal reaction and characterized using single crystal X-ray diffraction, Fourier transforms infrared spectroscopy, Thermogravimetric analysis, Powder X-ray diffraction, and Scanning electron microscopy. Both compounds exhibit good thermal and solvent stability.

These coordination polymers were used as heterogeneous Lewis acid catalysts for glycerol acetalization. The investigation has focused largely on the effect of reaction time and temperature, and catalyst to glycerol molar ratio. Optimal conditions for these two polymers included duration of 4 hours, a temperature of 50^o C, molar ratio of 1 to 10 catalyst to glycerol, and conversion percentage was 77% for $[Er_2(bpndc)_3(DMF)_2]$ polymer and 72% for $[Yb_2(bpndc)_3(DMF)_2]$ polymer. The catalysts leaching, stability, and recyclability were investigated. This study shows the potential role of the $[Er_2(bpndc)_3(DMF)_2]$ and $[Yb_2(bpndc)_3(DMF)_2]$ as heterogeneous Lewis acid catalyst for the glycerol acetalization.

Keywords: Coordination polymers; Lanthanides; Lewis acid catalysts; Acetalization

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The synthesis of α-diimine halide complexes using one-pot method for ethylene polymerization

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Abstract

A series of α-diimine halide complexes synthesized with a novel method. These complexes were prepared by the reaction of one-pot in which the ligand is catalyzed by an acid catalyzed condensation followed by direct addition of Nickel dibromide. Ethylene polymerizations catalyzed by these nickel α-diimine complexes activated by modified methylaluminumoxide (MMAO) were systematically investigated. Polymer molecular weight and resulting polymer microstructure were changed according to the catalyst structure modification and polymerization parameters and produced high molecular weight polyethylene.

Keywords: α-diimine halides complexes, one pot reaction, polymerization ethylene, symmetric catalysts.

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" Copper(II)-Silica fume Catalyzed Selective Synthesis of 1,8-dioxo-octahydroxanthenes: A Promising Approach towards Green and Efficient Organic Synthesis"

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Xanthenes and their derivatives have been a subject of significant interest lately, owing to their potential applications in diverse fields such as laser technology, pharmaceutical, and biological sciences. These chemical compounds have demonstrated various advantages, including but not limited to anti-inflammatory, antimicrobial, antiviral, and antitumor activities. Given their potential therapeutic benefits, promising candidates for drug development are currently being pursued. Numerous methods have been proposed in the scientific literature for synthesizing biologically relevant compounds, particularly 14-aryl-14H-dibenzo[a,j]xanthenes and 1,8-dioxo-octahydroxanthenes. Various catalytic structures such as metal salts, metal oxides, metal nanoparticles, carbon-based nanomaterials, and MOFs are utilized in these methods. Catalysts, while effective, can bring about practical issues like limited reusability, corrosion, and high cost. The synthesis of benzoxanthenone derivatives that are eco-friendly is gaining popularity. Scientists are developing green and reusable catalysts using simple and inexpensive materials to address sustainability and environmental safety concerns. Copper has emerged as a more favorable option among various metals due to its exceptional catalytic activity and relatively low cost. Numerous studies have confirmed that the collaboration between copper and diverse support materials can notably improve catalytic performance and simplify the separation process.

The use of Silica fume, a byproduct of silicon metal or ferrosilicon alloy production, as a high-performance catalyst has gained significant interest in recent years. Its amorphous structure, high surface area, and remarkable thermal and chemical stability make it an ideal support for metal doping, leading to enhanced catalytic activity. This research paper presents a practical and sustainable method for producing benzoxanthenones and xanthenes derivatives using Copper(II)-silica fume as an eco-friendly catalyst under mild conditions. The approach demonstrates a cost-effective and environmentally friendly alternative to traditional chemical synthesis methods.

In the performed reaction, an Aldehyde (1 mmol) was combined with dimedone (2 mmol) along with Copper(II)-Silica fume (40 mg) as a catalyst. The reaction mixture was then stirred in an ethanol solvent at a temperature of . It is worth mentioning that the catalyst produced through synthesis can be utilized for up to five consecutive runs without any notable decline in reaction efficiency.

Keywords: Xanthenes; Catalysts; Copper-silica fume.

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"Synthesis of 2-Amino-4H-Chromene Derivatives using Creatine-Functionalized Graphitic Carbon Nitride: A Promising and Efficient Catalyst"

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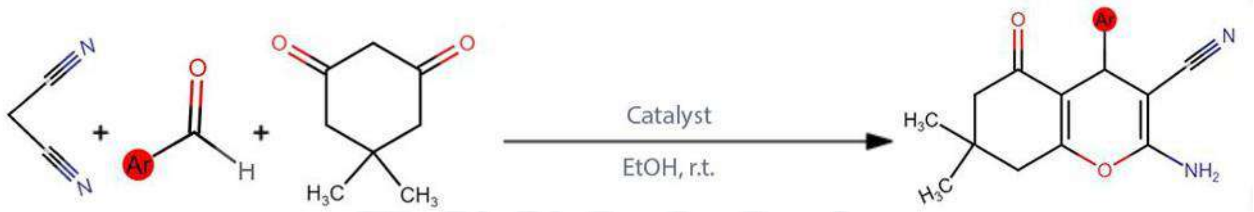
Oxygen-containing heterocyclic substances have garnered significant attention in various industrial applications, from cosmetics and pigments to medicine and biodegradable agrochemicals. Among these substances, 2-amino-tetrahydro-4H-chromene-3-carbonitrile is a promising candidate with its unique applications[1]. Researchers have employed various homogeneous and heterogeneous catalysts to synthesize these substances. These methods have limitations, such as long reaction times, high catalyst loading, tedious workup procedures, and low yields. In this regard, alternative approaches have been developed. For example, the functionalization of stable supports like silica NPs, graphene oxide, polymers, etc, along with an organocatalytic active site, has been reported. Bio-based creatine has been explored as a natural chemical substance for producing a variety of catalysts, owing to its ability to activate raw materials in both acid-catalyzed and base-catalyzed reactions. Having carboxylic and amine groups, it is regarded as a green and natural alternative for chemists who are interested in sustainable materials[2]. On the other hand, graphitic carbon nitride, as a solid support with a high surface area, demonstrated exceptional properties for the preparation of catalysts.

We have successfully developed a novel catalytic system by combining creatine with graphitic carbon nitride support through a 1,3-dibromopropane linker. This catalyst has been employed in a single-step, three-component condensation reaction of malononitrile, aldehyde, and dimedone to produce 2-amino-tetrahydro-4H-chromene-3-carbonitrile derivatives with high efficiency and selectivity. The reaction was performed by combining 1 mmol of dimedone, 1 mmol of aromatic aldehydes, and 1 mmol of malononitrile in 5 mL of ethanol with 0.04 g of the prepared catalyst. The results showed that the chromene derivatives were synthesized with an excellent yield of 85% up to 95%. Moreover, the catalyst remained effective for up to five consecutive runs without significantly declining reaction efficiency.

Keywords: 2-amino-4H-chromene derivatives; graphitic carbon nitride; creatine



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Preparation, identification and post-synthesis modification of Zn-Fe double layer hydroxide and investigation of its catalytic properties

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Layered double hydroxides (LDHs), also known as anionic clays or hydrotalcite-like compounds, are a class of nanomaterials that attained great attention as a carrier for drug delivery applications. In this research, the synthesis and identification of catalyst substrate Zn-Fe was studied. First LDH was synthesized by hydrothermal method. Epoxides are well known as one of the most valuable intermediates for the production of commercially important chemicals such as polyglycols, polyamides, polyurethanes and many other polymers, pharmaceuticals, food additives, epoxy paints, dye-stuffs, flavour and fragrance compounds, and non-toxic PVC-plasticizers and stabilizers. They are also valuable additives to lubricants and adhesives. morphology and structure of the prepared catalyst, by the methods, FTIR (Fourier Transform Infrared Spectroscopy), Gc Mas (Gas chromatography-mass spectrometry, SEM (Scanning electron microscopy) and XRD (powder X-ray diffraction) was performed. One of the most important reactions in organic chemistry is the epoxidation of alkenes. The catalyst Zn-Fe was used in the epoxidation reaction of alkenes. One of the advantages of using this catalyst over other catalysts is the good performance of high efficiency. The advantages of using this catalyst over other catalysts include good performance, high efficiency, short reaction time, economy and reusability.

Keywords: Layered double hydroxide, Epoxidation, epoxidation of alkenes, catalyst

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Evaluating on lactase enzyme immobilization in magnetic gel beads

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Enzymes are biocatalysts that catalyze biological reactions and have many applications in industry. Lactase is one of these industrial enzymes that is widely used in the milk and dairy industry and hydrolyzes milk sugar called lactose into glucose and galactose. Therefore, by using enzyme immobilization methods, their stability can be increased and they can be used several times, as well as reducing the isolation methods after that. Entrapment is one of the methods for enzyme immobilization that can be used according to the enzyme and the desired industry. In this method, enzyme is limited in a certain space and only the substrate and product are allowed to enter and exit. Various matrices are used for immobilization, and according to their needs and characteristics, the most suitable matrix should be chosen. Alginate is one of these matrices that has been considered due to its availability, cheapness, non-toxicity and biocompatibility. Also, in addition to the matrix, materials such as glutaraldehyde can be used to enzymes immobilization, which creates cross-links and improves enzyme immobilization. Glutaraldehyde also causes base stability and even increases thermal stability. Iron oxide nanoparticles are widely used in separation technology, protein immobilization, catalysis, medical and environmental sciences. In this research, the effect of adding glutaraldehyde and magnetic nanoparticles into calcium alginate beads and the immobilization amount and the activity of the immobilized lactase enzyme have been investigated. In the control case, calcium alginate beads were synthesized only with lactase enzyme, and the immobilization amount of the enzyme and its activity were obtained as 50.9 and 34.9%, respectively. By adding glutaraldehyde inside the beads, the immobilization amount and activity was obtained as 74.2 and 58.9%, respectively. In another case, the effect of adding magnetic nanoparticles to calcium alginate beads was examined, and in this case, the immobilization amount and activity were 79.4 and 55.3%, respectively. Also, in another experiment, the simultaneous effect of adding glutaraldehyde and magnetic nanoparticles was investigated, and in this case, the immobilization amount and activity was obtained as 76.84 and 13.82% respectively. According to the obtained results, it can be concluded that although the separate addition of glutaraldehyde and nanoparticle slightly increases the activity of the immobilized enzyme and immobilization amount of the enzyme, respectively, the simultaneous addition of both of them causes a sharp decrease in the activity of the immobilized enzyme. This sharp reduction could be because the simultaneous addition of glutaraldehyde and magnetic nanoparticles made the pores smaller and made it harder for the substrate and product to enter and exit the beads, and it may also have caused the enzyme to be positioned in such a way that the active site of the enzyme away from the substrate. Even the increase in hydrophobicity due to the addition of nanoparticles is one of the other reasons for reducing the activity of the immobilized enzyme, because it reduces the entry of the substrate into the beads.

Keywords: Enzyme immobilization; Lactase; Alginate; Glutaraldehyde; Entrapment; Magnetic gel beads.

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Photocatalytic removal of malachite green dye from aqueous solutions using nanostructures Ag-ZnO and UV irradiation

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Pollution of aquatic ecosystems by dyes is one of the most important issues in the environment, which requires providing effective and fast methods to remove these pollutants [1]. So far, various physical and chemical methods such as ozonation, membrane filtration, ion exchange, electrochemical methods and photochemical oxidation methods have been used to remove these pollutants from industrial effluents and aqueous solutions [2]. One of the most useful methods that does not cause secondary pollution in chemical treatment is advanced oxidation processes (AOPs) [3].

Malachite green dye is an organic compound that has wide industrial applications as a colorant and antimicrobial, especially in the aquaculture industry all over the world. The discharge of colored effluents containing green malachite into aquatic ecosystems has created very serious risks for human health and the environment [4].

In this research, the AOPs method was used in the presence of Ag-ZnO nanostructure as a photocatalyst to remove malachite green [5, 6]. A double-walled reactor was used and three ultraviolet lamps with a radiation wavelength of 254 nm and a total power of 24 watts were used vertically in the reactor, and experimental information was obtained after adjusting the pH and temperature of the solution and the concentration of oxidant and photocatalyst.

The progress of the reaction was followed by measuring the concentration by an ultraviolet-visible spectrophotometer in the desired time period, and the effects of temperature and different concentrations of photocatalyst and oxidant were also investigated.

The results show that after 90 minutes of exposureat, at a pH of about 5 and a temperature of 25 degrees Celsius and at the optimal concentrations of photocatalyst (100 ppm) and optimal concentrations of oxidant (100 ppm), 98.8% of the organic matter in the aqueous solution has been converted into inorganic compounds. The proposed path of decomposition is: decomposition of the conjugated structure, N-dimethylation reactions, hydroxyl addition reactions, removal of the benzene ring, and ring opening reaction and finally the mineralization of the green malachite compound (i.e. turning into water, carbon dioxide and compounds Nitrogen) [7]. The significant reduction of COD criterion up to 94% confirms the above results.

Keywords: Photocatalyst; green malachite Dye; ultraviolet light; Chemical Oxygen Demand (COD); Ag-ZnO Nanostructure.

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Photocatalytic decomposition of Bismarck brown dye in aqueous solutions using nanoparticles ZnO and hydrogen peroxide in the presence of UV light

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Azo dyes are widely used in various industries such as textile, pharmaceutical, food, cosmetics and printing industries. Currently, thousands of types of these colours are used and about half a million tons are produced worldwide [1]. Pollution of aquatic ecosystems by dyes is one of the most important issues in the environment, which requires providing effective and fast methods to remove these pollutants [2]. Until now, various physical and chemical methods have been used to remove these pollutants from industrial effluents and aqueous solutions [3]. One of the most useful methods that does not cause secondary pollution in chemical treatment is advanced oxidation processes (AOPs) [4].

Bismarck brown is an organic compound used in tissue staining and mucin monomer structures in cell membranes and cartilage. Bismarck Brown is an approved biological stain for microscopy, histology and cytology. It is also used in the textile industry. It is a special powder for coloring cellulose tissues, which is insoluble in acetone, benzene and carbon tetrachloride and slightly soluble in water. The aim of this study is to investigate the decomposition of brown bismarck in aqueous solutions using direct ultraviolet (UV) light irradiation in the presence of ZnO nanoparticles as a photocatalyst.[5]

In this research, a double-walled reactor was used and three ultraviolet lamps with a radiation wavelength of 254 nm and a total power of 24 watts were used vertically in the reactor, and the experimental information was obtained after adjusting the pH and temperature of the solution and the concentration of the oxidant and photocatalyst. The progress of the reaction was followed by measuring the concentration by an ultraviolet-visible spectrophotometer in the desired time period, and the effects of temperature and different concentrations of photocatalyst and oxidant were also investigated.

The results show that after 60 minutes of exposure, at a pH of about 6.5 and a temperature of 25 degrees Celsius and at the optimal concentrations of photocatalyst (200 ppm) and oxidant (200 ppm), 99% of the organic matter in the aqueous solution is converted into inorganic compounds. has been The significant reduction of the COD criterion confirms the above results. The test results showed that the decolorization of azo dyes is faster than the reduction of chemical oxygen demand (COD). The reason for the lower reduction of COD in the solution may be due to the accumulation of some products that resist mineralization [6].

Keywords: photocatalyst; Bismarck brown; ultraviolet light; ZnO nanoparticle; COD.

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Photocatalytic decolorization of Bismarck brown in aqueous solutions using TiO_2 nanoparticles in the presence of UV light

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Azo dyes are widely used in various industries such as textile, pharmaceutical, food, cosmetics and printing industries. Currently, thousands of types of these colors are used and about half a million tons are produced worldwide [1]. Pollution of aquatic ecosystems by dyes is one of the most important issues in the environment, which requires providing effective and fast methods to remove these pollutants [2]. Until now, various physical and chemical methods have been used to remove these pollutants from industrial effluents and aqueous solutions [3]. One of the most useful methods that does not cause secondary pollution in chemical treatment is advanced oxidation processes (AOPs) [4].

Bismarck brown is an organic compound used in tissue staining and mucin monomer structures in cell membranes and cartilage. Bismarck Brown is an approved biological stain for microscopy, histology and cytology. It is also used in the textile industry. It is a special powder for coloring cellulose tissues, which is insoluble in acetone, benzene and carbon tetrachloride and slightly soluble in water. The aim of this study is to investigate the decomposition of Bismarck brown in aqueous solutions using direct ultraviolet (UV) light irradiation in the presence of TiO_2 nanoparticles as a photocatalyst [5].

Titanium dioxide has wide applications, such as photodegradation of various pollutants, killing bacteria and killing tumor cells in cancer treatment. The presence of colored substances on the surface of titanium dioxide initiates light-sensitive processes. In these processes, the color compound(s) adsorbed on the titanium dioxide surface can absorb radiation in the visible range [6].

In this research, A double-walled reactor was used and three ultraviolet lamps with a radiation wavelength of 254 nm and a total power of 24 watts were used vertically in the reactor, and experimental information was obtained after adjusting the pH and temperature of the solution and the concentration of oxidant and photocatalyst

The progress of the reaction was followed by measuring the concentration by an ultraviolet-visible spectrophotometer in the desired time period, and the effects of temperature and different concentrations of photocatalyst and oxidant were also investigated.

The results show that after 90 minutes of exposure, at a pH of about 6.5 and a temperature of 25 degrees Celsius and at the optimal concentrations of photocatalyst (200 ppm) and oxidant (200 ppm), 96% of the organic matter in the aqueous solution is converted into inorganic compounds. The significant reduction of COD criterion confirms the above results.The test results showed that the decolorization of azo dyes is faster than the reduction of chemical oxygen demand (COD). The reason for the lower reduction of COD in the solution may be due to the accumulation of some products that resist mineralization.[7]

Keywords: photocatalyst; Bismarck brown; ultraviolet light; TiO_2 nanoparticle; COD.

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An Efficient Synthesis of 3,4-Dihydropyrimidin-2(1H)-Ones Catalyzed by a Novel Covalent organic framework under Solvent-Free Conditions

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The novel porous covalent organic framework was prepared through the condensation reaction of melamine and phthalic acid and Cadmium acetate was then incorporated into the COF through a straightforward post-treatment. The catalytic activity of Cd-COF was investigated in the one-pot three-component Biginelli-type reaction, involving a series of aldehydes, β-diketones, and urea. It exhibited excellent activity and selectivity, facilitating the synthesis of a diverse range of 3,4-dihydropyrimidin-2(1H)-ones under solvent-free conditions. The novel catalyst was characterized using FT-IR, SEM, EDS, PXRD, and TGA analysis. This protocol features an efficient catalyst, ease of workup, simple separation without chromatography, and the reusability of Cd-COF for four runs. These are important highlights of this process, and it will likely find a wide variety of applications in academic and industrial research.

Keywords: Covalent Organic framewor; heterogeneous catalyst; 3,4-Dihydropyrimidin-2-(1H)-ones (DHPMs); one-pot; solvent-free; Biginelli reaction;

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Synthesis of Cu(II)-SB/GPTMS@SiO_2@Fe_3O_4 nanocomposite as a reusable catalyst for the preparation polyhydroquinoline derivatives

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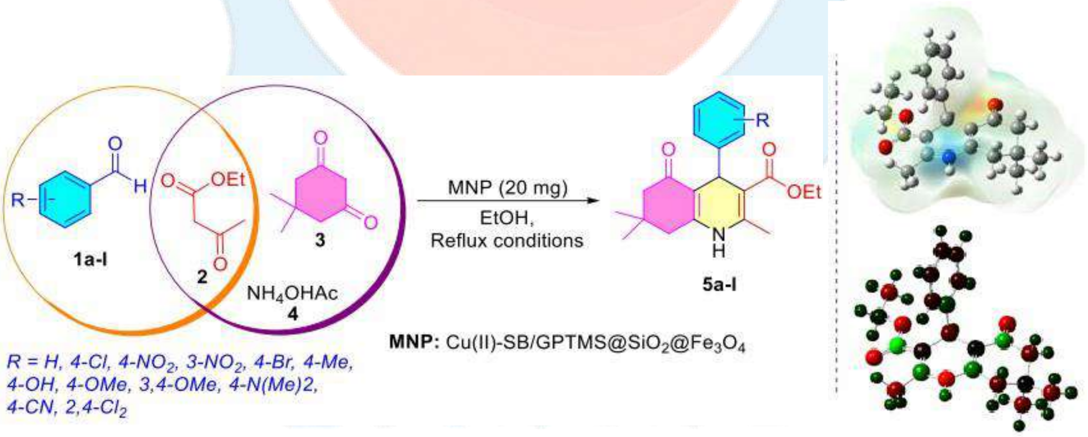
Magnetic nanomaterials have emerged widely as a powerful tool in the various fields such as environmental remediation, biotechnology, medical applications, pharmaceuticals, and the development of modern procedures for chemical synthesis. We synthesized a stable and reusable Schiff base complex of copper immobilized on core-shell magnetic nanoparticles [Cu(II)-SB/GPTMS@SiO_2@Fe_3O_4] by simple, efficient, and available materials. A variety of characterization analyses including fourier transform infrared (FT-IR), X-ray photoelectron spectroscopy (XPS), field-emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), Brunauer-Emmett-Teller (BET), thermogravimetric analysis (TGA), X-ray diffraction (XRD), vibrating-sample magnetometry (VSM), energy-dispersive X-ray spectrometry (EDX), and inductively coupled plasma (ICP) confirm that our synthesized nanocatalyst was obtained. After detailed characterization, the resulting nanocatalyst exhibited excellent catalytic performance for the explored catalytic reactions in one-pot synthesis of polyhydroquinoline derivatives by Hantzsch reaction of dimedone, ethyl acetoacetate, ammonium acetate, and various aldehydes in sustainable and mild conditions. The corresponding products is achieved in yields of 88-97% (Scheme 1).

Keywords: Cu(II)-SB/GPTMS@SiO_2@Fe_3O_4, Recyclable catalyst, Polyhydroquinoline



Scheme 1. Cu(II)-SB/GPTMS@SiO_2@Fe_3O_4 catalyzed the one-pot synthesis of polyhydroquinoline derivatives

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ZrFe2O4@SiO2@SO3H: a novel and efficient nanomagnetic catalyst for green synthesis of biologically active polyhydroquinoline derivatives

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Molecules that contain polyhydroquinoline structural scaffolds are N-containing heterocycles which are of great interest to organic chemists and biologists. Polyhydroquinoline structural scaffolds which are known as calcium channel blockers have emerged as one of the most important class of drugs used for the treatment of cardiovascular and Alzheimer's diseases. Besides, recovery and reusability of catalysts are important issues to be discussed in modern catalysis research especially in organic synthesis. The concept of magnetically recoverable catalysts has been rapidly developed in recent times. Magnetic separation is an efficient strategy for the rapid separation of catalysts from the reaction medium. Also, an alternative to time-, solvent-, and energy-consuming separation techniques. In this study, we focused on the fabrication, surface-modification and characterization of nanomagnetic materials and their application, as magnetically recoverable catalysts, in the synthesis of polyhydroquinoline structural scaffolds..

Keywords: Hantzsch reaction; Magnetic nanoparticles; Multicomponent reaction

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Matrix of Zirconocene Chloride on Magnetite-reduced Graphene Oxide: A Heterogeneous catalyst for One-pot Three-component Synthesis of Tetrahydrobenzo[b]pyrans and Dihydropyrano[3,2-c]chromenes

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Abstract: The present paper describes the synthesis and characterization of the functionalized magnetite reduced graphene oxide (rGO@Fe_3O_4) with zirconocene dichloride as rGO@Fe_3O_4@$ZrCp_2Cl_2$. The prepared magnetic nanomaterial was characterized by Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), thermogravimetric analysis (TGA), vibrating sample magnetometer (VSM), inductively coupled plasma optical emission spectroscopy (ICP-OES) and mass spectrometry (MS). This new heterogeneous nanocatalyst showed the perfect catalytic activity towards synthesis of tetrahydrobenzo[b]pyran and dihydropyrano[3,2-c]chromene derivatives through multicomponent reaction of dimedone or 4-hydroxycoumarin, malononitrile and aromatic aldehydes in polyethylene glycol 400 (PEG-400) at 100 °C. The influence of the amount of nanocatalyst, varying temperature of the reaction and the kind of solvent on the rate of condensation reaction was investigated. Recovery and reusability of the applied nanocatalyst was examined for five consecutive cycles without the significant loss of its catalytic activity.

Keywords: Dihydropyrano[3,2-c]chromene, Dimedone, 4-Hydroxycoumarin, Malononitrile, rGO@Fe_3O_4@$ZrCp_2Cl_2$, Tetrahydrobenzo[b]pyran

Electrodeposition of nickel-cobalt on graphite rod as an efficient electrocatalyst for hydrogen and oxygen evolution reactions

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Abstract: We need energy to get by in our daily lives. The population is growing faster than ever, which means that energy production needs to increase. By 2035, estimates indicate that there will be over 8.7 billion people on the planet, meaning that an extra 1.6 billion people would need energy[1]. Use of renewable energy sources, including hydrogen, has increased due to the depletion of fossil fuel supplies and the ensuing damage to the environment[2]. Electrolysis, which comprises oxygen and hydrogen evolution processes on the anode and cathode faces, respectively, is one of the most widely used methods for producing hydrogen. The slow rate of water electrolysis is caused by the several interactions that must occur between the electrode surfaces, ions, and electrons as a result of these processes[3]. The NiCo-based electrocatalytic enhancements for the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) are the focus of this study. Utilizing cyclic voltammetry on a graphite rod substrate, the synthesis method offers a singular one-step electrochemical process. By adjusting variables including cycle counts, scan speeds, and Ni:Co concentration ratios, the ideal circumstances for efficient catalyst manufacturing were found. The main conclusions show that there may be hydrogen evolution reaction (HER) activity on the improved Ni-Co coating on graphite rod, with minor over voltages of -255.3 and -402.9 mV at current densities of 10 and 100 mA. cm^{-2}, respectively. Moreover, the generated Ni-Co electrocatalyst exhibits good performance in the oxygen evolution process (OER) by requiring just 380 mV overpotentials to operate at a current density of 10 mA. cm^{-2}. Its high stability, activity, and enhanced kinetics are highlighted in the paper, which attributes these qualities to novel microstructures, a binder-free electrodeposition process, and the synergistic effects of Ni and Co. This study presents a highly effective catalyst for electrolysis and demonstrates an inexpensive and straightforward synthesis strategy, opening the way to scalable and sustainable energy generation.

Keywords: Ni-Co; Electrocatalyst; Hydrogen evolution reaction; Oxygen evolution reaction; Water splitting

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Study of photodegradation of Rhodamine B using silver doped titanium dioxide magnetic composite

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In this research, dandelion nanoparticles of titanium dioxide and magnesium ferrite have been synthesized using hydrothermal methods in two steps. In addition, silver was doped as a metal element in different weight percentages (1, 2, 3, 4 and 5% by weight) via the photoreduction method on $TiO_2/MgFe_2O_4$ composite. One of the most important innovations of the current research was the simultaneous investigation of silver doping and the formation of a heterojunction structure between TiO_2 and $MgFe_2O_4$ in order to increase the performance of the photocatalyst in the photodegradation of Rhodamine B under irradiation of 250w Osram mercury vapor lamp. The characteristics of the prepared photocatalysts were determined by the analysis of FESEM, XRD, DRS, and VSM. Also, based on FESEM and XRD, it was observed that the TiO_2 photocatalyst nano-dandelion structure was well formed and $MgFe_2O_4$ was loaded. On the other hand, based on the VSM analysis, the optimal photocatalyst has a favorable magnetic property, which has led to easy separation and recovery of the photocatalyst using a simple magnetic field. In addition, According to DRS analysis the highest light intensity was obtained by this composite, and the band gap energy for the composite was reduced. Finally, the photodegradation rate of Rhodamine B for the $TiO_2/MgFe_2O_4/2Ag$ photocatalyst after 2 hours at a concentration of 10 ppm under mercury vapor lamp light was 94.7%, which is the best performance compared to the fabricated photocatalysts.

Keywords: TiO_2, Magnetic photocatalytic, Heterojunction structure, doping silver, Rhodamine B;

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Catalytic activity of manganese porphyrin supported on magnetic nanoparticles in the degradation of organic dyes

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Industrial dyes represent a major group of hazardous, toxic and resistant organic pollutants with undesirable effects on the human health and aggravates the shortage of water because of releasing huge amount of colored and pollution in the environment [1]. Recently, catalytic oxidation processes have been widely used for the transformation of the pollutants into more functional and nontoxic compounds [2] and scientists are working hard to develop novel and economically sustainable catalytic systems for the degradation of textile wastewaters. Among different catalytic systems, synthetic and bio-inspired metalloporphyrin complexes have been extensively used as effective catalysts for the oxidation reactions, because of its excellent ability to oxidize a wide range of the substrates such as water pollutants under the mild conditions [3].

In this study, *meso*-tetrakis(4-carboxyphenyl) porphyrinato-manganese (III) acetate was stabilized on magnetic nanoparticles and was evaluated using different methods such as thermal gravimetry (TGA), scanning electron microscope (FE-SEM), transmission electron microscope (TEM). Vibrating sample magnetic analyzer (VSM), X-ray diffraction pattern (XRD), infrared spectroscopy (FT-IR) and electron spectroscopy (UV-Vis). The amount of manganese stabilized on the substrate was determined by atomic absorption spectrometer (AAS). The synthesized catalyst was evaluated in the degradation of organic dyes. In the next step, in order to compare the effect of the central metal on the activity of the catalyst, the oxidative degradation of methyl orange and methylene blue, were investigated in the presence of hydrogen peroxide in aqueous medium and the effect of various parameters which may affect the catalytic efficiency were optimized. In addition, the prepared nanocatalyst showed little deactivation with time, was easily recovered by an external magnet, and could be reused at least five times with no significant loss in the activity.

Keywords: Manganese porphyrin; Organic dyes, Catalyst, Magnetic nanoparticles, Degradation

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Synthesis, Characterization, Comparative Study and Catalytic Activity of the Modified MNPs for Green Oxidation of Sulfides

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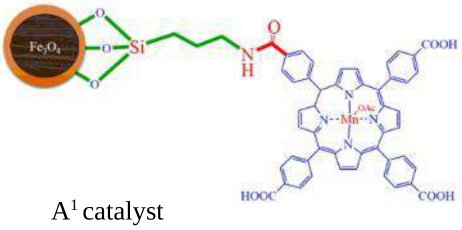
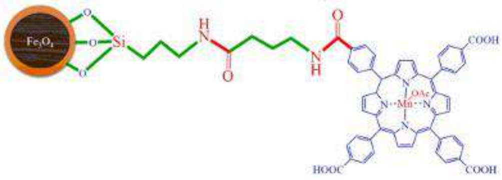
It is concerned that oxidation of sulfides is a worthwhile topic through industry and environment due to the pollution that of sulfide. Controlling the selective oxidation of sulfides in order to produce the correspond sulfoxides and sulfones have been attracted researcher's interest, as well. Among the oxidation reaction products, sulfoxides are more beneficial, whose acts as various chemically and biologically active intermediates and therapeutic agents. According to environmental issues, toxic or polluter products such as sulfides must be eliminated, especially from the environment. During decades, Eco-friendly oxidant such as urea hydrogen peroxide (UHP) attained much attention in the industry and environment. High oxidizing power, economical friendly and abundance make UHP a valuable oxidant for oxidation reaction [1-3].

In the following research, *meso*-tetrakis(4-carboxyphenyl)porphyrinatomanganese (III) acetate (MnTCPP) was immobilized onto the surface of two various modified magnetic nanoparticles (MNPs) via different linkages ($Fe_3O_4@SiO_2-NH_2$-MnTCPP(OAc) (A^1 catalyst) and $Fe_3O_4@SiO_2$-NHCO-NH_2-MnTCPP(OAc) (A^2 catalyst)). The prepared catalysts were identified by AAS, UV-Vis, FT-IR, VSM, FE-SEM and TEM techniques. The prepared magnetic nano-catalysts with different linker lengths were participated in the comparative study of oxidation of sulfides with urea hydrogen peroxide (UHP) and acetic acid (HOAc as co-oxidant). The higher rate of oxidation reaction and reusability were achieved in the oxidation reaction of 2-(ethylmercapto)-ethanol (≥99%) and thiophene (≥99%) in the presence of catalyst with longer linker length (A^2 catalyst) in ethanol at ambient temperature. Besides, Turnover number (TON) of catalytic reaction using A^2 catalyst was highly enough to consider the catalyst as an efficient material to oxidize the sulfides. Moreover, Both A^1 and A^2 catalysts have accomplished 5 runs of recycling without significant decrease in their activity.

Keywords: Manganese porphyrin; Sulfides, Catalyst, Magnetic nanoparticles, Oxidation



A^1 catalyst



A^2 catalyst

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The silica-coated magnetite nanoparticle has been coated by tris(8-quinolinolato)iron that was coordinatedly immobilized via NH2. Fentonlike catalyst with selection for the clean oxidation of sulfides: Fe3O4@SiO2-FeQ3.

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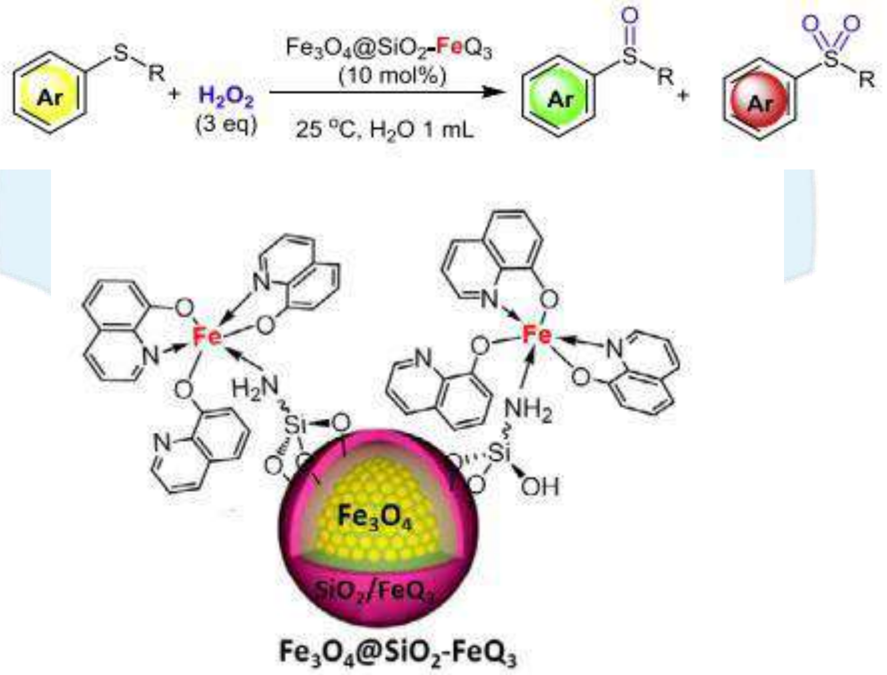
An environmentally-friendly process has been designed to convert aromatic organic sulfides into sulfones by employing H2O2 as a catalyst and NH2-coordinately immobilized tris(8-quinolinolato)iron on silica-coated magnetite (Fe3SiO6). The sulfide oxidation method's catalytic activity demonstrated that this atom-economical protocol produced high yields of different sulfones and enable the sulfide function reaction to proceed at mild circumstances, limiting the sulfide from being overoxidized to sulfoxides. The Fe3O4@SiO2-FeQ3 catalysts can be separated magnetically and maintained stable for seven consecutive runs without exhibiting any discernible decrease in activity.



Scheme 1: Optimal reaction conditions for the oxidation of sulfur compounds

Keywords**:** “Fe3O4@SiO2-FeQ3”, “aromatic organic sulfides”

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PET waste is green appraised and transformed into functionalized .Cu-MOF for the catalytic reduction of 4-nitrophenol

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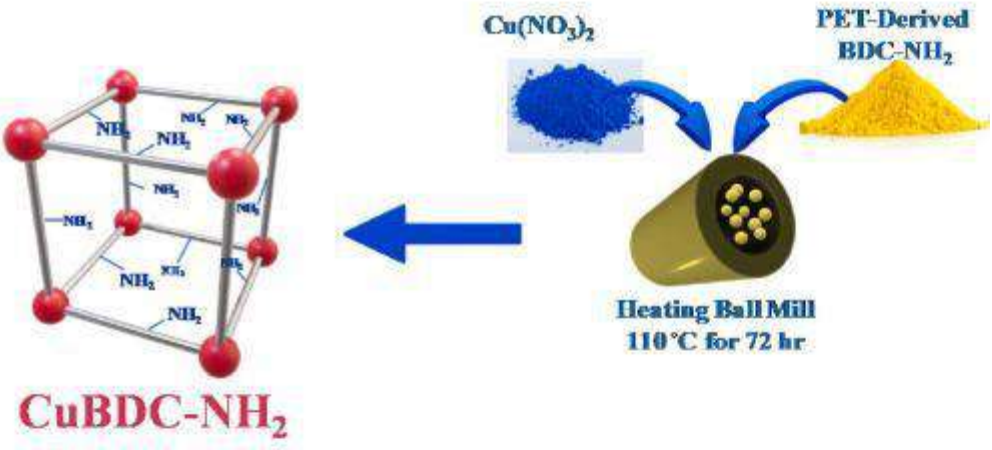
Metal-organic frameworks (MOFs) are extremely popular functional materials due to their flexible compositions, high porosity, and extensive surface area. Still, their large-scale uses are hindered by the costly precursors and complicated synthesis process[1,2]. Here, an innovative environmentally friendly method for synthesis Cu-based MOF has been created using a solvent-free mechano-synthesis method, with the use of benzenedicarboxylate (BDC) produced by consumed polyethylene terephthalate (PET) as the linker[3].



Scheme 1: Illustration of the synthesis.

Keywords: “PET”, “polyethylene terephthalate” , “Metal-organic frameworks”

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pyrido[2,3-d:5,6-d$^{/}$]dipyrimidinesare synthesized using $CuFe_2O_4$ a magnetically recoverable nanocatalyst solvent-free

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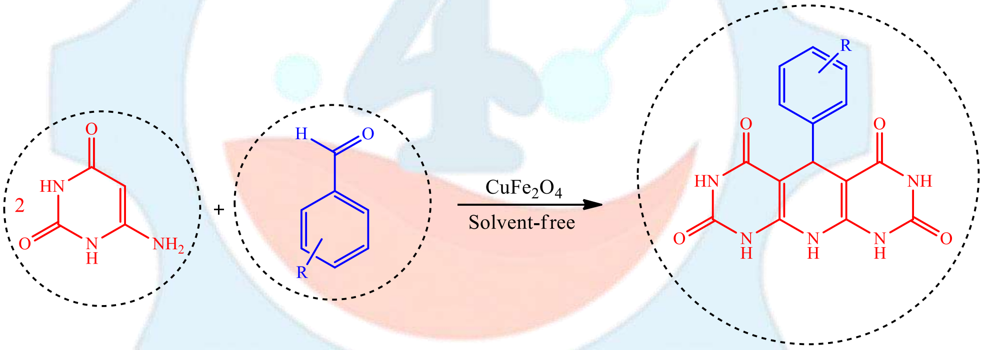
Abstract

Due to their extensive range of biological and therapeutic properties and inclusion in the natural goods' structures, heterocyclic compounds are a significant class of organic molecules. Pyrido[2,3-d:5,6-d$^{/}$]dipyrimidines . are a specific family of heterocyclic substances that have a pyrimidine ring in their structure. Derivatives of Pyridodipyrimidine have numerous biochemical effects, including antitumor and blood pressure treatment. [1,2]. In this study, we reported pyrido[2,3-d:5,6-d$^{/}$]dipyrimidine compound synthesis solvent-free using $CuFe_2O_4$ NPs.(Scheme).



Scheme: Synthesis compound pyrido[2,3-d:5,6-d$^{/}$]dipyrimidine solvent-free using CuFe2O4 NPs

Keywords: “Multicomponent reactions”, “Heterogeneous catalys”, “$CuFe_2O_4$ magnetically nanoparticles”

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A new adsorbent composite fabricated by waste paper and reduced graphene oxide aerogel for removal of crystal violet dye

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The presence of dye in the water stream leads to unexceptional effects on living life. Small-scale to large-scale industries such as tanneries, food, cosmetic, textile, and medicinal sectors consume dyes globally with the production of 1,000,000 tons all over the world. The coloration of dyes is imparted due to the presence of chromogen and chromophore groups. Among several natural and synthetic dyes, azo group dyes have been known highly carcinogenic due to amine and benzidine emissions. In addition to this, hazardous dye molecules last longer in the environment because of their non-biodegradability. Therefore, it is needed to eradicate dye molecules from wastewater before discharging the stream into the environment with long and short-term effects [1]. Apart from dye pollution, paper is the third largest industrial pollutant for ecosystem health. Paper comprises a network of plant fibers laid down as a flat sheet that is made from a suspension of plant tissues in water, known as pulp. The plant fibers of waste paper are reusable for six to seven times. Hence, the demand for recyclable waste paper is rapidly increasing in the global market [2]. Graphene-based aerogels, the known lightest three-dimensional structures, have been a longstanding of interest due to their unique and exceptional features such as remarkable adsorption capacity, specific surface area, electrical conductivity, thermal resistance, and high mechanical strength. In this context, one of the most appropriate building precursors to fabricate aerogel structures is graphene oxide (GO), the oxidized derivative of graphene sheets. Thanks to the oxygen-containing functional groups of GO sheets at both basal plans and edges, these functional sheets can react non-covalently and covalently with different compounds to generate new materials with specific efficiency and tailored applicability. According to the colloidal stability of GO sheets, applying the hydrothermal process, and reducing the oxygen-containing functional groups, the individual GO sheets are cross-linked reduced graphene oxide (rGO) aerogel is formed. This multifunctional structure with a high surface area can act as an excellent adsorbent substrate to design and fabricate advanced and newly discovered compositions. In this research work, a new composite was designed and synthesized based on the extraction of cellulosic fibers from waste paper, its combination with graphene oxide sheets, in-situ reduction process, and formation of cellulosic fiber/reduced graphene oxide aerogel composite. Following characterizing its chemical and structural features (FT-IR, EDX, FE-SEM, XRD, TG analyses), this new resulting aerogel composite is a promising adsorption material for the removal of crystal violet through electrostatic interactions between the aerogel and the cationic dye for environmental engineering.

Keywords: Paper waste, Reduced graphene oxide aerogel; Adsorbent composite, Dye removal, Crystal violet

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Scheme 1 Synthesis process of cellulosic fiber/rGO aerogel composite adsorbent and its adsorption activity for removal of crystal violet dye.

Application of efficient $ZrO(NO_3)_2.2H_2O$ catalyst in the synthesis of new ferrocenyl imidazo[1,2-a]pyridine-3-amine derivatives

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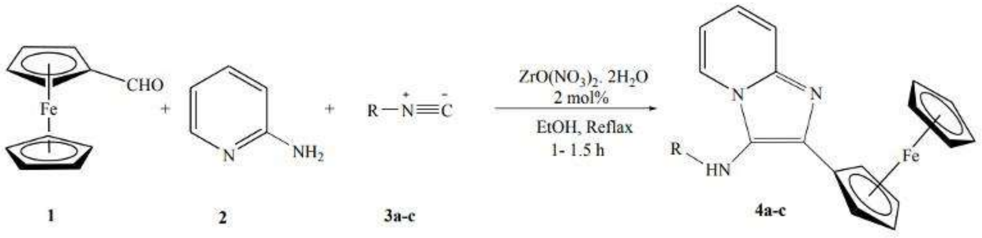
Nitrogen-based heterocyclic chemistry is a fundamental aspect of organic chemistry. Imidazo[1,2-a]pyridine derivatives belong to this category and have numerous biological properties, such as anti-inflammatory, antiviral, antibacterial, antifungal, antiprotozoal, etc.[1]. Several methods for the synthesis of imidazo[1,2-a]pyridines have been described in the literature [2], one of which is Groebke- Blackburn-Bienaymé reactions (GBBRs)[3]. GBBRs are types of multicomponent reactions among 2-amino azine, an aldehyde, and an isocyanide in the presence of various catalysts [4]. In this work, we reported the synthesis imidazo[1,2-a]pyridine derivatives from the multicomponent reaction of ferrocenecarboxaldehyde **(1)** , 2-aminopyridine **(2)**, and isocyanides (**3a-c**) using $ZrO(NO_3)_2.2H_2O$ as a catalyst under reflux conditions in EtOH. The advantage of the present study is the use of a very small amount of the catalyst $ZrO(NO_3)_2.2H_2O$ and a short reaction time with high yielding. This catalyst is reclaimable for synthesizing compounds. All of the compounds were characterized by FT-IR and ^{1}H-NMR, ^{13}C-NMR spectroscopy method.



R: Cyclohexyl, Benzyl, tert- Butyl

Figure 1.Scheme of the reaction

Keywords: Groebke- Blackburn-Bienaymé reactions; Imidazo[1,2-a]pyridine; $ZrO(NO_3)_2.2H_2O$

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Photochemical-assisted synthesis of Ce@$FeTiO_3$ nanocomposite for photocatalytic degradation of rhodamine-B under visible light irradiation

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Due to the rapid growth of society, there are significant environmental issues, such as the contamination of drinking water by residues like dyes or agrichemicals. Currently, there is a strong interest in the use of photocatalytic materials for energy and environmental applications. One such material that has been extensively researched is ferrite titanate ($FeTiO_3$), which shows potential for ecological use. The recovery and collection processes following photocatalytic reactions are more efficient with magnetic photocatalysts. $FeTiO_3$ is a semiconductor with a band gap of 2.5-2.9 eV and is well-known for its magnetic properties [1-3]. In this research, $FeTiO_3$ was utilized as an affordable and eco-friendly catalyst for the photocatalytic degradation of rhodamine-B dye. The $FeTiO_3$ nanoparticles were synthesized using the sol-gel method. To enhance the structure and optimize the photocatalytic activity, cerium atoms were incorporated onto the surface and within the structure using a combination of photochemical and sol-gel techniques. The catalytic properties were evaluated through various analyses, including XRD, SEM-EDS, TEM, UV-Vis, and DRS, to assess the morphology, optical properties, and structure of the nanoparticles. The results of relevant analyses confirm the synthesis of titanate ferrite in the nanoscale range. The study involved a systematic analysis of the effect of Ce concentrations in $FeTiO_3$, initial solution pH, and reusability. The presence of cerium on the perovskite surface of the electron-hole combination causes a delay and improvement in the photocatalytic performance of the sample, resulting in faster degradation of pollutants. By adding cerium to the perovskite structure and adjusting its band gap, the photocatalytic activity increases due to the unique properties of cerium such as different electronic structure and redox coupling. Optimum conditions for rhodamine-B photocatalytic degradation were achieved with 0.2% Ce content, 0.02 g/L nanocomposite dosage, and a pH of 7. Collecting the catalyst with a magnet and reusing it after several consecutive cycles, as well as the degradation of more than 70% of the pigment in the presence of visible light due to the presence of cerium atoms on the surface of FeTiO3, shows the promising potential of this nanostructure.

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SiO2/TiO2/g-C3N4 nancomposite membrane photocatalytic activity under UV light

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The presence of organic pollutants, such as dyes, pharmaceuticals, and industrial wastes, in the environment has become a global concern due to their stability and slow decomposition. These pollutants, along with heavy metals, have been found to have detrimental effects on human health, including the potential to cause cancer, kidney failure, Angiocardiopathy, high blood pressure, and other diseases. As a result, it is crucial to urgently develop effective methods for treating wastewater. One widely used approach is the use of titanium dioxide (TiO_2) semiconductor photocatalysis, which has high catalytic activity. However, the photocatalytic performance of TiO_2 is limited due to its high intrinsic recombination rate of holes and electrons as well as its wide band gap energy of approximately 3.2 eV. One of the most effective ways to address the limitations of TiO_2 is by incorporating it with other semiconductors. Recent studies have shown that TiO_2 can be combined with graphitic carbon nitride (g-C_3N_4), which has a band gap of 2.7 eV. However, the combination of inorganic TiO_2 and heterogeneous g-C_3N_4 still suffers from low efficiency, greatly limiting its practical use in environmental remediation. To improve the performance of this photocatalytic system, silica (SiO_2) can be added as a component, increasing the surface area and stability of the catalyst [1-3]. In this study, a three-component nanocomposite of SiO_2/TiO_2/g-C_3N_4 was prepared using a simple ultrasonic method and evaluated for its ability to degrade methyl orange (MO) under ultraviolet (UV) light. Nano-sized mesoporous TiO_2 and SiO_2 are dispersed onto the g-C_3N_4 layers. Pollutant adsorption occurs on the SiO_2 nanoparticles, while the photocatalytic reaction is driven by the valence band (VB) of TiO_2 and the conduction band (CB) of g-C_3N_4. The samples were characterized using an X-ray diffractometer, transmission electron microscope, energy dispersive X-ray spectrometer, UV-visible spectroscopy, and Fourier transform infrared spectroscopy. Photodegradation studies demonstrate that a nanocomposite with a SiO_2/TiO_2 (1:1) molar ratio of 0.02 g on the carbon nitride surface can decompose more than 85% of a 10 ppm MO solution in just 10 minutes under UV light. The high degradation percentage of methyl orange in such a short time, as well as the degradation of other cationic and anionic dyes by this nanocomposite, showcases its excellent performance as a photocatalyst.

Keywords: SiO_2/TiO_2/g-C_3N_4 nanocomposite; methyl orange; UV-light photocatalysis; wastewater

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$FeTiO_3$/g-C_3N_4 hybrid architectures as visible-light-driven photocatalyst for Acid red 88 degradation

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Industrialization has led to a significant increase in the amount of toxic waste being released into our environment and water systems. This has resulted in water pollution, which poses a threat to both human health and the well-being of other living beings. In order to combat this issue, the use of photocatalytic degradation has emerged as an efficient and environmentally friendly method for breaking down organic pollutants in water. In recent years, there has been a growing interest in compounds with a perovskite structure (ABO_3), particularly those based on titanium, due to their long lifetime, wide band gap, excellent catalytic activity, and high chemical and optical stability. The crystal structure of perovskite and its distortion play a crucial role in the splitting of optical charge carriers, which can be manipulated to alter the band gap and absorption of visible light. This allows for the band edge energy to be adjusted to meet the specific requirements of different photocatalytic reactions. Iron titanate ($FeTiO_3$) is a commonly used iron-based perovskite oxide with a favorable band gap of 2.5-2.9 eV. It is recognized as a crucial catalyst for the photocatalytic degradation of organic pollutants due to its unique antiferromagnetic properties. However, pure $FeTiO_3$ has poor catalytic activity due to fast charge recombination. To address this issue, it is effective to construct hybrid systems by coupling $FeTiO_3$ with other photocatalysts, which can accelerate efficient charge separation and transfer [1-3]. In this study, graphitic carbon nitride (g-C_3N_4) was obtained through thermal pyrolysis and used to prepare $FeTiO_3$/g-C_3N_4 hybrid structures using an ultrasonic method. The structural, morphological, and optical properties of the synthesized nanocomposite were characterized using XRD, FTIR, VSM, and UV-visible techniques. Various weight percentages of a nanocomposite $FeTiO_3$/g-C_3N_4 were synthesized. The hybrid architecture, created by combining 100 mg of $FeTiO_3$ with 20 mg of g-C_3N_4, demonstrated excellent photocatalytic degradation of 50 ppm of acid red 88 under visible light. The use of this $FeTiO_3$/g-C_3N_4 hybrid catalyst increased the photocatalytic efficiency of pure $FeTiO_3$ from 43.05% to 86.86%. This improvement can be attributed to the proper band alignment and heterogeneous transfer mechanism, which prevent the recombination rate of photo-excited charge carriers. The effects of the initial concentration of the pollutant (10, 50, and 100 mg/L) were investigated in the presence of 0.02 g of catalyst. The results showed that the incorporation of $FeTiO_3$ particles with g-C_3N_4 sheets significantly enhanced the photocatalytic properties of $FeTiO_3$ under various conditions.

Keywords: hybrid systems; perovskite; photocatalytic degradation; $FeTiO_3$

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Ionic liquid $[HNMP]^{+}$ $[HSO4]^{-}$, An Efficient And Recyclable Catalyst For The Synthesis Of Isoxazolone Derivatives *via* Eco-Friendly Condition

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Abstract

Recently ionic liquids (ILs) have grown interest in diverse areas of chemistry; because of considerable interest as eco-friendly reaction solvent and catalyst in the organic synthesis. They exhibit significant properties such as negligible vapor pressure, broad liquid range, non-flammability, adequate ionic conductivity, potentially recyclable properties and capacity to dissolve a variety of organic and inorganic solids. Acidic ionic liquids have been employed in divergent areas due to their fascinated physical and chemical properties. $[HNMP][HSO_4]$ is also a brønsted acidic ILs has successfully used in various organic reactions such as cyclocondensations reactions. A simple and efficient protocol for the one-pot synthesis of 3-methyl-4-((3-aryl-1-phenyl-1*H*-pyrazol-4-yl)methylene)isoxazol-5(4*H*)-one derivatives has been described by environmentally benign, one-pot three component condensation of substituted 1,3-diaryl-1*H*- pyrazole-4-carboxyaldehyde, β-keto ester and hydroxyl amine hydrochloride in the presence of ionic liquid $[HNMP][HSO_4]$ as a catalyst in water. These derivatives have been synthesized by conventional, ultrasound and microwave irradiation methods. The combination of ionic liquid with ultrasound as well as microwave irradiation makes the protocol fascinating and environmentally benign. In addition, it has several benefits such as simple work-up procedure, clean reaction profile, short reaction time and good yields.

Keywords: ionic liquid, eco-friendly catalyst, isoxazolone, ultrasound, microwave

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Zeolite Catalyzed Synthesis of Imidazole Derivatives

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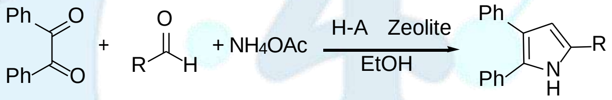
Acid-catalyzed organic transformations are essential in chemical and industrial processes. Among these catalysts, zeolites which are generally defined as porous crystalline aluminosilicates, are highly efficient materials used in the chemical industry. Acid sites occurring on zeolites make these microporous solids interesting materials for heterogeneous catalysis of carbon-carbon and carbon-nitrogen bond forming reactions. [1] In this work, HA zeolite as a heterogeneous catalyst with a mild acidic property can catalyze trisubstituted imidazoles. Imidazole derivatives are a group of structure that have a unique chemical complexity.

Imidazole nucleus, nitrogen-containing heterocyclic ring, is very practical and versatile in its construction and can be considered a rich source of chemical diversity. Imidazole acts in extremely important processes for the maintenance of living organisms, such as catalysis in enzymatic processes. Imidazole-based compounds with antibacterial, anti-inflammatory, antidiabetic, antifungal, antioxidant, antitumor, anticancer, antidepressant and many others make these compounds very important in the most diverse works. [2-4]

In the present article, we have developed a mild, efficient and environmentally benign method for the synthesis of imidazole derivatives. This research shows the use of substituted 1,2-diphenylethane-1,2-diones (benzils), substituted aldehydes and ammonium acetate under thermal conditions, with the aim of optimizing the construction of 2,4,5-trisubstituted imidazoles. The reactions are simple and fast, as illustrated in the Scheme below, which uses the system with EtOH and HA zeolite as catalyst.



Keywords: Imidazole; HA zeolite; Benzils; Heterogeneous catalysis.

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Hydroxy Sodalite Zeolite Catalysed Synthesis of N'-Hydroxybenzenecarboximidamide Derivatives

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The field of organic catalysis over zeolites and related microporous materials has shown enormous international expansion, since the early 1960s. Increasing assemblage of zeolite structures has been explored multiplicity of new reactions; also understanding the catalytic chemistry and structure-reactivity relationships has shown dramatic growth. There are many applications for zeolites, such as, adsorption of As (V) [1], cracking of oil to produce liquid hydrocarbon fuel [2], valorization of agro-industrial waste [3] and immobilization of enzymes in biocatalytic processes. Among these crystalline zeolites hydroxy sodalite can act as water adsorbing agent in purification of water/1,1-dimethylhydrazine mixture, dehydrating agent in conversion of alcohols to ethers or alkenes [4]. Amidines are an important class of bioactive compounds found in a wide variety of natural products. These compounds are important pharmaceutical intermediates which widely used as antibiotics, anti-inflammatories and anthelmintic agents [5]. Also, amidine derivatives can be used as starting materials for synthesis of heterocyclic compounds; thus, efficient strategies for their preparation are in great demand.

In this research, synthesis of *N*-hydroxybenzimidamides were reported by hydroxy sodalite as an efficient, excellent, readily available and very inexpensive catalyst. Applying benzonitriles, hydroxyl amine hydrochloride and hydroxy sodalite zeolite in ethanol under reflux conditions gave the products in high yields. Environmentally benign and easy work-up of reactions are the other advantages of this method.

Keywords: *N*-hydroxybenzimidamides; Hydroxy sodalite zeolite; hydroxyl amine hydrochloride.

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Synthesis of Fe304@Si02@GPTMS/Schiff base Cu(II) nanocomposite as a heterogeneous catalyst for the Knoevenagel condensation

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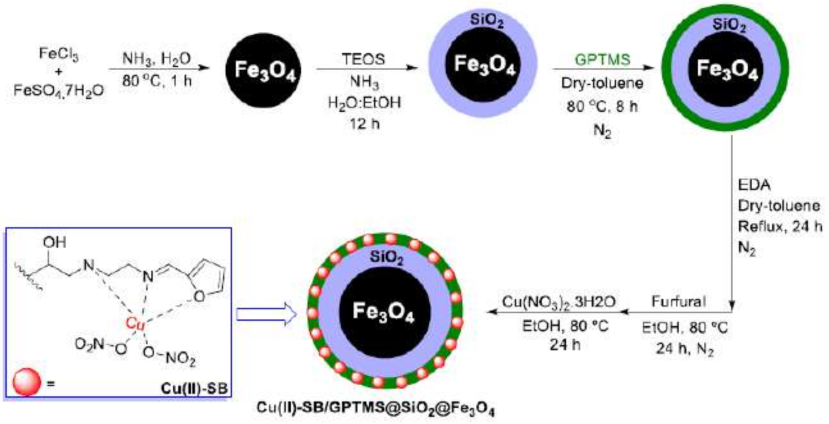
The Schiff base complex of copper immobilized on core-shell magnetic nanoparticles [Cu(II)- Schiff base /GPTMS@Si02@Fe304] was prepared via chemical modification of Fe^O^ nanoparticles with a thin layer of SiO: and then was uniformly enveloped with GPTMS to give GPTMS@Si02@Fe304. After synthesis of GPTMS@Si02@Fe304, they were reacted by means of EDA to give EDA/GPTMS@Si02@Fe304. In continuation, EDA/ GPTMS@,Si02@Fe304 was treated with furfural in an aqueous solution of ethanol under reflux conditions to afford Schiff base/GPTMS@Si02@Fe3C>4. Finally, treating this material with Cufhh^EGFEG in ethanol under reflux conditions resulted in the formation of a magnetically separable Cu(II)- Schiff base/GPTMS@Si02@Fe304 nanocatalyst according to Scheme 1. The physiochemical properties of the nanocatalyst prepared were investigated by using Fourier transform infrared (FT-IR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Brunauer-Emmett-Teller (BET), X-ray diffraction (XRD), vibrating-sample magneto-metry (VSM), energy dispersive X-ray spectrometry (EDX), and inductively coupled plasma (ICP) analyses. The catalytic movement of the synthesized nanocatalyst underwent successful investigation in the Knoevenagel condensation through malononitrile as well as various aldehydes in H2O as a green solvent at room temperature. The high efficiency, short reaction time, ecofriendly properties, and easy workup can be considered the major benefits of the current method.

Keywords: Fe304@Si02@GPTMS/Schiff base Cu(II); Magnetically recoverable catalyst; Heterogeneous catalysis



Scheme 1. Preparation of the Schiff Base Complex of Copper on Epoxy-Modified Fe^C4@SiCL MNPs

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The effects of Ti^{3+} self-doping on the photocatalytic properties of titanium dioxide synthesized by the sol-gel method

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Abstract

The technology of water purification employing TiO_2 photocatalyst, extensively studied and commercialized in many developed countries of the world. However, due to its wide bandgap, it can only be activate under UV irradiation and has high charge recombination and low carrier separation efficiency. In this research, the sol-gel method used for the synthesis of self-doped titanium dioxide. Using of the self-doped TiO_2 can protect the chemical and physical stability of this material during the photocatalytic process. In addition, this material has a lower bandgap and absorbs more light energy. It is very effective for repeating the photocatalytic process due to the non-entry of external material into the structure of the material, because during photocatalytic process, doping materials may separate from the structure of the TiO_2. The synthesis of self-doped TiO_2 is easier and does not have the Complexity of doping with metallic and non-metallic materials. To achieve a satisfactory result from this photocatalyst material, it depends on the several factors, including the type of pollution, the appropriate synthesis method, and the suitable light source, which must be in balance with each other. This research focuses on the modification of the UV-TiO_2 photocatalytic process, using self-doping to improve the photocatalytic activity for dye degradation. At first TiO_{2-x} anatase self-doped with Ti^{3+} synthesized, and then various analyzes including XRD, EDS, UV vis, Raman, FTIR, PL were performed on the sample and finally it was used to degrade methylene blue dye. From this research, we concluded that TiO_2 self-doped with Ti^{3+} clearly increased the intrinsic oxygen vacancies in TiO_2 crystals at the same time. Presence of oxygen vacancies and structural defects can trap electrons and holes, and prevent their recombination and have an improvement on the photocatalytic process.

Keywords: Photocatalyst; titanium dioxide; dye degradation; pollutant; anatase; synthesis

Biosynthesis of palladium nanoparticles using Dorema aucheri leaf extract: highly efficient catalyst for Mizoroki–Heck cross-coupling reaction

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In this work an environmental-friendly approach for the fabrication of a heterogeneous palladium nanocatalyst was reported using Dorema aucheri leaf extract, a straightforward technique, and with no additional surfactant, stabilizing and capping agents. Various spectroscopic techniques, including field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), and energy-dispersive X-ray spectroscopy (EDS) microanalysis were used to confirm the formation of bio-synthesized Pd NPs. Highly dispersed palladium nanoparticles applied as a recyclable and reusable catalyst to achieve palladium (II)-catalyzed Mizoroki–Heck reaction of n-butyl acrylate with various aryl halides under solvent-free conditions. Additionally, the isolation of the nanoparticles did not require a complicated and lengthy workup procedure. Also, the nanocatalyst was recycled by a simple filtration and reused for five runs successfully.

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Global economic outlook of the catalyst industry and Challenges of catalyst supply and production in Iran

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Catalysts are used in any chemical reaction where optimal speed and conditions are desired, and it speeds up only reactions that are carried out thermodynamically. In fact, they create the role of accelerating chemical reactions that may normally take years to complete and cause a significant increase in productivity and production of chemical products. The importance of the production of catalysts is such that it can be said that some chemical reactions are not carried out in practice without their presence and no product is produced. In this research, it is intended to deal with the concepts and applications of the catalyst along with its general classification. In this regard, attention and examination of global statistics on the amount of consumption of various types of catalysts by consumer countries can show a comprehensible picture for those involved in the catalyst industry. The purpose of this research is to analyze and investigate the global catalyst market and identify the major catalyst producing companies. It is hoped that by examining the challenges in the industry and estimating the total volume of the refinery and petrochemical catalysts market and quantitative and qualitative analysis of the catalyst industry market, we can take an effective step in the development of the domestically produced catalysts market. Considering the existence of actual and potential refinery and petrochemical complexes Inside the country, the annual consumption value of catalyst in Iran is about 700 million dollars. The contribution of petrochemical catalysts is approximately 450 million dollars per year due to the number and variety of processes used. Refinery complexes of the country also consume 250 million dollars of catalyst per year despite the low complexity factor and inappropriate processing pattern. Statistics show that only 10% of the domestic market value of Catalyst is 700 million dollars, provided by domestic companies. Forecasting the total nominal capacity of current and future consumption of catalysts needed by the country, such as petrochemical polymer, non-petrochemical polymer, petrochemical and gas refinery until 1404, 28 thousand 839 tons per year and its total price based on current and future consumption is 692 million It is dollars.

concepts and applications of catalyst| global economy of catalyst| economy and challenges of catalyst production in Iran

Cu(I) complexes supported with dihydrobis(2- mercapto-benzimidazolyl)borate and phosphine ligands as a homogeneous catalyst for synthesis of 2H-indazoles

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A series Cu(I) complexes containing dihydrobis(2-mercapto benzimidazolyl)borate and phosphine co-ligands were synthesized and their catalytic activity was investigated in synthesis of 2H-indazoles. These complexes were experimented as catalyst system and among them a Copper(I) complex containing tricyclohexylphosphine co-ligand, [Cu(Bb)(PCy3], displayed superior catalytic activity.

The introduced ligands are advantageous due to their strong σ-donating ability, nontoxicity and the ease of their handling process. The selected catalyst permitted the successfully preparation of 2H-indazoles in PEG-200 in relatively short reaction times.

These catalysts were prepared by reacting copper iodide with sodium precursor (NaBb) [Bb=dihydrobis(2-mercapto-benzimidazolyl)borate in methanol in the presence of selected phosphine co-ligands (PPh3, ,PPh2Me, PPh2Py, PCy3). All of the resulting Cu(I) complexes were formed as predominantly a single monomeric isomer and were characterized using a combination of 1H, 13C{1H} and 31P{1H} NMR spectroscopy.

Keywords: 2H-indazoles, Cu(I) complexes, catalyst.

Green synthesis and characterization of spinel manganate nanoparticles by tragacanth gel and studies of its photocatalytic activity for wastewater treatment

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The innovative approach of green synthesis utilizing plant extracts introduces an eco-friendly and cost-effective methodology for nanomaterial production, diverging from traditional, environmentally harmful practices prevalent in both laboratories and industries. This method emphasizes the use of phytochemicals found in plants, which vary in composition but generally contain beneficial compounds such as alkaloids, steroids, phenols, terpenoids, flavonoids, saponins, quinones, and coumarins. By leveraging these natural compounds, the green synthesis technique replaces hazardous chemicals and solvents with safer, plant-derived phytochemicals and water-based solutions, establishing a sustainable and environmentally benign protocol for nanomaterial synthesis [1].

Manganese spinels, represented by the general formula AB_2O_4, where A and B are metal cations, are notable for their diverse applications across electronics, catalysis, and energy storage due to their unique structural and magnetic properties. These materials, including variations like $MnFe_2O_4$, $LiMn_2O_4$, and $ZnMn_2O_4$ exhibit a range of magnetic behaviors, from ferromagnetic to antiferromagnetic, depending on their specific compositions. This makes them valuable for use in magnetic storage, spintronic devices, and as MRI contrast agents [2].

In the realm of catalysis, which plays a pivotal role in modern technology and science, nanocatalysts have emerged as a promising area of research, offering the potential to enhance catalytic performance while reducing the reliance on expensive materials. Specifically, magnetic nanocatalysts have garnered significant attention for their applications in environmental remediation, such as the removal of pollutants and mitigation of toxicity. These nanocatalysts, characterized by their large magnetoresistance, high Curie temperatures, and efficient magnetic properties, are particularly useful in treating polluted water and subsurface environments due to their economic viability, ease of recovery, and reusability [3].

Our study delves into the plant-mediated biosynthesis of magnetic nanomaterials, spotlighting the utilization of biosynthesized nanoparticles as green nanocatalysts in the transformation of catalytic organic chemicals and the removal of organic dyes from wastewater. These synthesized magnetic nanoparticles demonstrate excellent photocatalytic performance in degrading organic pollutants under natural conditions and pH levels. We have developed $Zn_xMg_{1-x}MnFeO_4$ magnetic nanoparticles (MNPs) through a straightforward, green sol-gel method. The characterization of these nanomaterials employed various techniques, including XPS, XRD, and TEM, among others, to evaluate their photocatalytic activity specifically in the rapid decolorization of Reactive Blue 21 dye. Remarkably, these nanoparticles maintain their efficiency and structural integrity even after multiple recycling processes, showcasing their potential for sustainable environmental applications.

Keywords: Photocatalyst, Reactive Blue 21, Spinel

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Synthesis of new nano magnetic semiconductors based on camphoric acid and their applications in photodegradation of pollutants

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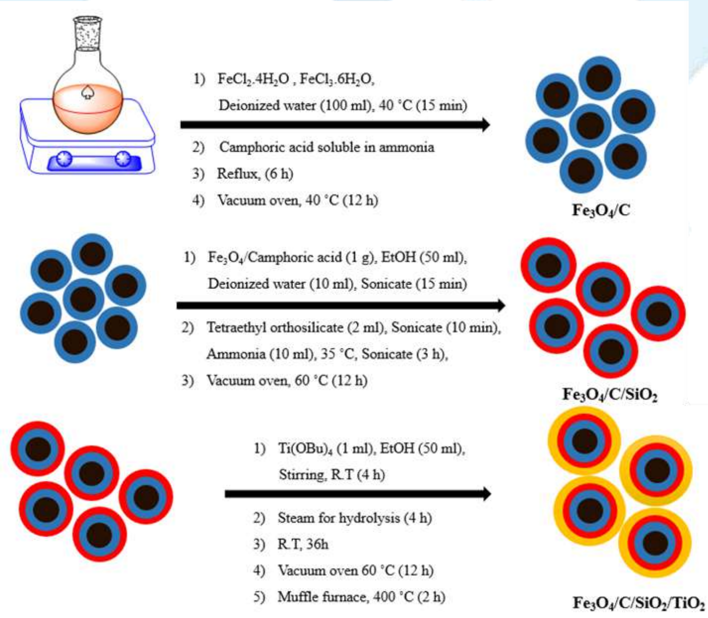
In this investigation, camphoric acid was used for the first time as a carbon source for synthesizing $Fe_3O_4/C/SiO_2/TiO_2$ and $Fe_3O_4/C/TiO_2$ nano-semiconductors. These nano-photocatalysts were used for the photodegradation of PCB in transformer oil (Askarel) and PCB 138 in aqueous solutions under visible light irradiation and without hydrogen peroxide. Interestingly, in addition to the extraction degradation method, direct degradation was also carried out. also, we observed camphoric acid significantly reduced the band gap and these reduced band gap semiconductors (2.10 eV) were characterized by field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), N_2 adsorption-desorption isotherm analyzes and vibrating sample magnetometer (VSM). The high photocatalytic performance compared to $Fe_3O_4/C/TiO_2$ and P25 in direct and indirect (extraction-degradation) degradation as well as the convenient magnetic recovery are the main advantages

Keywords: Camphoric Acid, Photodegradation, Askarel oil, PCB 138, $Fe_3O_4/C/SiO_2/TiO_2$, Visible light



Scheme1: Synthesis of $Fe_3O_4/C/SiO_2/TiO_2$

Bi-functional Cu-P@Ni-Mn-Se 3D structure on nickel foam as an electrocatalyst for hydrogen production

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As the population grows, the consumption rate of limited fossil fuel resources rises, causing pollution. Therefore, hydrogen fuel has been introduced as a sustainable and clean energy carrier, making it the fuel of the future[1].

During alkaline water electrolysis, two half-reactions take place: the hydrogen evolution reaction (HER) at the cathode and the oxygen evolution reaction (OER) at the anode. The OER is a slow reaction that requires a significant overpotential to occur. According to theoretical studies, to decompose water and produce hydrogen, a potential of 1.23V is needed. A cost-effective and highly efficient electrocatalyst could be a potential solution. In recent years, various methods have been developed for synthesizing stable and efficient electrocatalysts using elements found on Earth[2].

Noble metals such as platinum and their alloys are highly effective due to their low Tafel slope and overvoltage close to zero. However, their high price and limited availability restrict their usage. As an alternative, non-noble metals are used as a more cost-effective electrocatalyst that is highly efficient and stable. Therefore, non-noble metals are a suitable replacement for noble metals[3, 4].

In this study, a nanocomposite, Cu-P@Ni-Mn-Se, was synthesized electrochemically on nickel foam and used as an efficient electrocatalyst for HER. First, copper-phosphide (Cu-P) was deposited on the nickel foam using the chronopotentiometry technique, followed by the deposition of nickel-manganese-selenium (Ni-Mn-Se) on it using the chronoamperometry technique. The electrode surfaces were analyzed using X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDS), field-emission scanning electron microscopy (FESEM), and cyclic voltammetry (CV) methods. To improve the efficiency of the electrode for HER, we have optimized the crucial parameters. The proposed electrode is cost-effective using non-noble metals, has a high surface-to-volume ratio, a large number of active sites, and good electrical conductivity due to the deposition method.

Keywords: Hydrogen production; Hydrogen evolution reaction; Electrocatalyst; Water splitting

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Preparation of Industrial Catalyst for Amino acid Synthesis

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Abstract

The present invention relates to the production of industrial Homogeneous catalysts with heterocyclic Alcoholic organic compound by reacting formaldehyde and ammonia.The reaction between formaldehyde solution and ammonium hydroxide solution results in a mildly alkaline solution that widely employed in the production of amino acid.

Key Word: Alpha halo acid, Catalyst, Amino Acide,

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Zeolite Catalyzed Synthesis of Imidazole Derivatives

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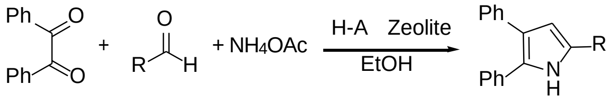
Acid-catalyzed organic transformations are essential in chemical and industrial processes. Among these catalysts, zeolites which are generally defined as porous crystalline aluminosilicates, are highly efficient materials used in the chemical industry. Acid sites occurring on zeolites make these microporous solids interesting materials for heterogeneous catalysis of carbon-carbon and carbon-nitrogen bond forming reactions. [1] In this work, HA zeolite as a heterogeneous catalyst with a mild acidic property can catalyze trisubstituted imidazoles. Imidazole derivatives are a group of structure that have a unique chemical complexity.

Imidazole nucleus, nitrogen-containing heterocyclic ring, is very practical and versatile in its construction and can be considered a rich source of chemical diversity. Imidazole acts in extremely important processes for the maintenance of living organisms, such as catalysis in enzymatic processes. Imidazole-based compounds with antibacterial, anti-inflammatory, antidiabetic, antifungal, antioxidant, antitumor, anticancer, antidepressant and many others make these compounds very important in the most diverse works. [2-4]

In the present article, we have developed a mild, efficient and environmentally benign method for the synthesis of imidazole derivatives. This research shows the use of substituted 1,2-diphenylethane-1,2-diones (benzils), substituted aldehydes and ammonium acetate under thermal conditions, with the aim of optimizing the construction of 2,4,5-trisubstituted imidazoles. The reactions are simple and fast, as illustrated in the Scheme below, which uses the system with EtOH and HA zeolite as catalyst.



Keywords: Imidazole; HA zeolite; Benzils; Heterogeneous catalysis.

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Application of novel core–shell hybrid nanomaterials [Cu(l-proline)$_2$] complex modified magnetic UiO-66-NH$_2$(Zr) in the synthesis of henry reaction

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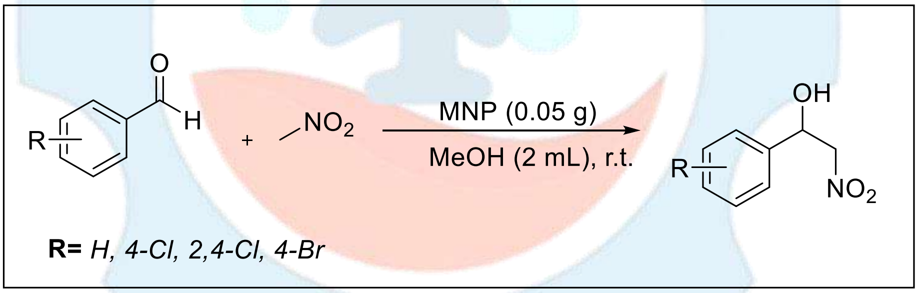
The essential need for today's methodologists is to design innovative approaches in organic synthesis to increase the environmental conservation by following the green chemistry principles [1-2]. Due to the importance of nanoparticles and MOFs, we synthesized the [Cu(l-proline)$_2$] complex modified magnetic UiO-66-NH$_2$(Zr) metal organic framework, and characterized and confirmed by Fourier transform infrared (FT-IR), X-ray photoelectron spectroscopy (XPS), field-emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), Brunauer–Emmett–Teller (BET), thermogravimetric analysis (TGA), X-ray diffraction (XRD), vibrating-sample magnetometry (VSM), energy-dispersive X-ray spectrometry (EDX), and inductively coupled plasma (ICP) analyses. The silica layer stabilizes the Fe_3O_4 core, and the chelation of Zr^{4+} by the -OH groups in the silica layer drives the growth of Zr-MOFs on the surface of Fe_3O_4. The as-prepared catalyst was employed in a study of the Henry reaction-type condensation of nitromethane and various benzaldehyde in MeOH at room temperature (Scheme 1). Upon completion of the reaction, the magnetic catalyst can be conveniently and efficiently recovered from the reaction mixture through the use of an external magnet and then reused in the next run. The results have revealed that the recovered catalyst does not significantly lose its activity after 8 cycles.



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Scheme 1: Synthesis of henry reaction catalyzed by MNP

Keywords: Magnetic nanoparticles; Heterogeneous catalysis; Henry reaction

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Green synthesis of ZnO-TiO2 nano photocatalyst doped with Fe(III) ion for wastewater treatment Contains dyes in the pharmaceutical industry

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Abstract

Dyes have become the main cause of water pollution in various industries such as pharmaceuticals, textiles, food, cosmetics and hygiene. The annual production of paint waste is estimated to be approximately 105 tons and more than 100,000 known types of paint are used in the industry. This study investigates the photocatalytic degradation of water pollutant using a newly synthesized ZnO−TiO2 nano-photocatalyst doped with iron ions. The nano-photocatalyst is prepared through a green method using bitter olive seeds and a sol-gel method for doping iron ions. The XRD, FE-SEM, TEM, BET, and EDX characterizations show that the nano-photocatalyst is successful with a particle size of 60 nm and a specific surface area of 187 m2 g−1. Response surface methodology and central composite design are used to optimize the photocatalytic degradation of reactive dyes in synthetic and industrial wastewater. The optimal conditions were found to be initial dye concentration of 10 mg L−1, nano-photocatalyst dose of 0.5 mg L−1, contact time of 85 min, and pH of 6.

Keywords: catalyst, nano photocatalyst,sol-gel, green synthesis

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Extraction of nanosilica from rice husk and inveistigation of nanosilica addition effects cement propentiey

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Abstract

The improvement and high efficiency of raw materials for cement-based constructions and the preservation of natural resources have been a constant challenge for today's society. For this purpose, the use of nanotechnology has received wide attention in recent years. The purpose of this research is to study the role of nanotechnology in the cement industry through improving the properties and recycling of an agricultural waste in order to preserve the environment and create added value. For this purpose, at first, nanosilica was extracted from rice husk, which is an agricultural waste and millions of tons of this waste are produced and burned in the world and Iran. The rice husk after removing metallic and mineral impurities was burnt in the furnace and white colored nano-silica was extracted from the ash of the rice husk through several stages, and by seveal washing with acids. The structure of extracted nano-silica was confimmed through X-ray techniques. The obtained nano-silica had of high purity and amorphous structure. In the following, silica nanoparticles were added to cement and had positive effects on cement properties such as compressive and flexural strength, setting time, matrix and cement density, which were all due to the particle size, high specific surface area of nanoparticles and pozzolanic activity of nanosilica.

Keywords: Rice husk; Synthese; Agricultural waste; Nanosilica; pozzolanic; Cement

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Designing of More Efficient Homogeneous or Heterogeneous Catalytic Systems Based On Hard Soft Acid and Base Theory

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More than 85% of the chemical processes in both lab and industry need a catalyst or a combination of two or more active catalytic species to afford a reasonable yield. Hence, both homogeneous or heterogeneous catalytic systems have found a vital role in the chemical and related industries.[1] Therefore, tremendous interest has been focused on designing of more efficient homogeneous or heterogeneous catalytic systems. This will result in not only more academic achievements and economic benefits but also make our planet safer for present and future generations.[2-10] Although designing of new catalyst may be occurred based on random, experience of experts in the field or some known theories, however classification of different catalytic systems based on Hard Soft Acid and Base (HSAB) Theory has received less attention. In this lecture, different homogeneous or heterogeneous catalytic systems based on HSAB Theory would be discussed to give more insight for designing of more efficient homogeneous or heterogeneous catalytic systems in both lab and industry.

Keywords: Homogeneous Catalysis; Heterogeneous Catalysis; Hard Soft Acid and Base (HSAB) Theory; Chemical Industry; Green and Sustainable Chemistry.

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Engineering Amino-Functionalized Metal-Organic Frameworks with Tailored Pore Size and Surface Chemistry for Enhanced Photocatalytic Reduction of Uranium under Visible Light Irradiation

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The elimination of uranium (U) from nuclear wastewater is crucial for the preservation of the environment due to its high level of toxicity and radioactivity. The reduction of U(VI) to U(IV) is widely regarded as an effective technique for the elimination of U(VI) from wastewater [1]. This approach is based on the distinction in solubility of U ions in its various valence states. The photocatalytic reduction of U(VI) has attracted considerable attention in the literature due to its simplicity, efficiency, and environmentally–friendly nature when compared to alternative reduction methods [2]. Metal-organic frameworks (MOFs), composed of metal ions/clusters and functionalized organic linkers [3], have emerged as effective photocatalysts for U reduction. These materials possess distinct advantages such as high surface area, well-defined molecular building blocks, stability, functional groups, and effective active sites [4]. The present study focuses on the development and application of NH_2-MIL-101(Cr) as a functionalized MOF, for U photoreduction using visible light. The amino ($-NH_2$) groups on the organic linker act as Lewis bases, possessing lone pair electrons that can form coordinate bonds with uranyl (UO_2^{2+}) ions. This interaction effectively confines the uranyl ions, demonstrating NH_2-MIL-101(Cr) superior performance in U(VI) removal compared to MIL-101(Cr) in both adsorption and photocatalysis. Consequently, the presence of $-NH_x$ groups serves as U(VI) confinement sites and significantly increase the reduction potential of U(VI).

Keywords: Nuclear wastewater; Uranium photoreduction; Functionalized metal-organic framework; Lewis base; Confinement sites.

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New MIL-53(Fe)/NiAl-LDH Thin Film as Effective Electrocatalyst of Oxygen Evolution Reaction

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Abstract

The electrocatalytic water splitting process includes two half-reactions: the oxygen evolution reaction (OER) and the hydrogen evolution reaction (HER) [1]. During the OER, the electrocatalyst facilitates the oxidation of water molecules to generate oxygen gas and protons. Researchers are constantly working towards developing efficient and cost-effective electrocatalysts for widespread water splitting application, which is crucial for advancing clean and sustainable energy systems [2].

Recently, metal-organic framework (MOF) nanoarchitectures have been developed, featuring ultra-large surface areas, tunable nanostructures, and excellent porosities. Proved to be promising materials for the development of highly active one's catalysts for electrochemical water splitting [3]. Many MOFs and MOF-derived electrocatalysts have been reported in recent years. Cu- and Cobased MOFs generally work well in electrocatalytic HER applications, while Fe-, Co-, and Ni-based MOFs can be used as highperformance OER catalysts. In MOF-derived electrocatalysts, HER catalysts mainly include metals, alloys, carbon materials, singleatom catalysts, transition metal carbides, phosphides, and sulfides (especially molybdenum and tungsten sulfides). For OER, MOFderived catalysts mainly include transition metal oxides/chalcogenides and metal phosphides [4].

In this paper, MIL-53(Fe) and NiAl-LDH were prepared via a facile solvothermal process, then MIL-53(Fe)/NiAl-LDH/NF and NiAl-LDH/MIL-53(Fe)/NF thin films were fabricated on nickel foam substrate (NF) using layer-by-layer (LBL) electrophoretic deposition technique. The synthesized composites as new water-splitting electrocatalysts were characterized by XRD, SEM, FTIR, and EDAX techniques. MIL-53(Fe)/NiAl-LDH/NF shows excellent oxygen evolution reaction (OER) activity in alkaline electrolytes with required overpotentials of 150, 220, and 320 mV to achieve current densities of 20, 50, and 100 mA cm^{-2}, respectively, and long-term stability for at least 20 h. This work can provide new insights arena for designing the LBL synthesized compounds of MIL53(Fe)/NiAl-LDH/NF and NiAl-LDH/MIL-53(Fe)/NF as new high performing OER electrocatalysts.

Keywords: MIL-53(Fe)/NiAl-LDH/NF; NiAl-LDH/MIL-53(Fe)/NF; Electrocatalysts; Oxygen evolution reaction; layer-by-layer.

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Experimental Study of the synthesis gas production using a nanophotocatalyst method in aqueous phase

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Abstract

Increasing global demand for energy is mainly supplied by fossil fuels, increasing concerns about the long-term availability of energy resources, global warming and the greenhouse gas emissions. The use of hydrogen as a fuel is a promising resource to overcome all the concerns caused by environmental pollution and reducing fossil reserves. However, more than 90 % of the hydrogen produced in the world is obtained from fossil fuels. During these processes, a large amount of carbon dioxide is released. Most of the produced hydrogen is consumed at the production unit. Only a small part of the produced hydrogen is used as an energy carrier, however with the development of technology, it will be possible to use it in various industries, including transportation, so that hydrogen is used as the fuel of the future. One of the alternative sources of fossil fuels for hydrogen production is water, that the method is completely renewable. Water can be divided into hydrogen and oxygen using different technologies. The usual method for this work is the electrolysis process. The production of hydrogen, economically and as an efficient method is limited in this method. A better and more appropriate method is direct fission in one step without using electric current. Photocatalytic production of hydrogen is a method that can be used to produce of oxygen and hydrogen. An ideal technique for green hydrogen production is water breakdown using a photocatalyst and sunlight .Applying the method economically depends on the development of semiconductor photocatalysts with a very large contact surface with suitable activity and stability.

In the experimental work, hydrogen is produced from CuCrO/ TiO_2 nanophotocatalyst method in methylene blue solution. In addition, the method of making nanoparticles of titanium dioxide (TiO_2), copper chromate (CuCrO) and combined photocatalyst of copper chromate/titanium dioxide (CuCrO/ TiO_2) is investigated. Then, the advantages of using a combined photocatalyst for hydrogen production have been investigated, experimentally. The crystalline phase and material structure, morphology and chemical composition were tested and analyzed using XRD, SEM/EDS and TEM/EDS measurements. The analyses show that a composite nanophotocatalyst has been formed.

The experimental results show that the Suspension sample B with a concentration of 0.5 g/l of copper chromate has the best photocatalytic activity and a degradation efficiency of 85.3%, about 1.14 times (i.e 14% higher) that of titanium dioxide (74.6%). The degradation efficiency increased from 0 to 0.5 g/liter of copper chromate concentration by 74.6% to 85.3%. The increased degradation efficiency can be attributed to the p-n heterogeneous layers between copper chromate nanoparticles and titanium dioxide nanorods by spin coating method. This catalytic method can be important due to the reduction of greenhouse gas emissions and environmental effects in order to produce a clean fuel.

Keywords: Nanophotocatalyst, Titanium oxide, copper chromate, synthesis gas, green hydrogen, methylene blue

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Fabrication of highly efficient photocatalysts based on TiO2 QDs for nitrogen photofixation

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One of the essential elements in the periodic table is nitrogen, which constitutes 78% of the earth's atmosphere. Nitrogen is the basic element of proteins, nucleic acids, and many important nitrogenous compounds. However, due to the triple bond within N_2, it needs more energy to be broken in ordinary conditions. Hence, nitrogen fixation has attracted numerous attention from researchers worldwide. Recently, the use of heterogeneous photocatalysts has been proposed as an effective solution for the production of ammonia, as one of the solar energy conversion processes, under mild conditions. Among various semiconductors, titanium dioxide (TiO_2) has been widely used as a photocatalyst due to its high photochemical stability, non-toxicity to the environment, and cost-effectiveness. However, considering poor visible-light absorption and high recombination of electron-hole pairs, significant research are carried out to prepare nanocomposites based on TiO_2 with high performances under visible light. Although the conduction band of TiO_2 is negative enough to reduce N_2 to ammonia, as the TiO_2 particles become smaller, the reducing and oxidizing power of this semiconductor increases, leading to more photocatalytic activity. Furthermore, TiO_2 quantum dots (QDs) have a higher surface area than pristine TiO_2, which leads to superior efficiency in photofixation by adsorbing and activating more nitrogen molecules. Therefore, we are trying to fabricate efficient photocatalysts for nitrogen photofixation using TiO_2 QDs. In these regards, very recently, we synthesized photocatalysts like TiO_2QDs/Bi_2O_3/$NaBiS_2$, TiO_2QDs/brown TiO_2, and TiO_2 QDs/Fe_3S_4 nanocomposites and applied them for simulated solar-light-induced nitrogen photofixation reaction [1-3]. The integration of TiO_2 QDs with Bi_2O_3/$NaBiS_2$, brown TiO_2, and Fe_3S_4 leads to the formation of hetero/homojunctions, which enhances the segregation of charge carriers and diminishes the electron-hole recombination [4]. Moreover, the mentioned nanocomposites have a much higher specific surface area than TiO_2 QDs photocatalyst. The increase in surface area is accompanied by an increase in active sites, and as a result, the transfer of nitrogen molecules to the surface increases, because the active sites are places to electron transfer from the photocatalyst to the adsorbed nitrogen molecules. As a result, the amount of ammonia production over TiO_2QDs/Bi_2O_3/$NaBiS_2$, TiO_2QDs/brown TiO_2, and TiO_2 QDs/Fe_3S_4 nanocomposites has increased significantly compared to the pure components. In the present paper, we will discuss about the advantages of these photocatalysts, and the future perspective of our research group.

Keywords: Photocatalytic N_2 fixation; TiO_2 QDs; Solar energy conversion; NH_3 photogeneration.

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Gold Nanoparticle Synthesis in the Presence of Polyphenolic and Flavonoid Compound as a Green Catalyst

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Nanotechnology has witnessed remarkable progress due to the development of novel synthesis methods for nanoparticles. Among these, green synthesis using plants has emerged as a sustainable and eco-friendly approach. This research explores the potential of plant-mediated synthesis for gold nanoparticles (AuNPs).

In this procedure, green synthesis of AuNPs involves the reduction of gold ions using plant extract or phytochemical derived from plant. This method offers numerous advantages, including its environmental friendliness, cost-effectiveness, and scalability. Notably, plant-mediated synthesis utilizes plant waste or by-products, making it a resource-efficient approach [1].

Plants are an abundant and diverse source of biomolecules that play crucial roles in AuNP synthesis. Polyphenols, flavonoids, alkaloids, and terpenoids are among the key secondary metabolites present in plants, which act as reducing and stabilizing agents during nanoparticle synthesis [2]. Different plant species and extracts harbor unique compositions, enabling the production of AuNPs with varying sizes, shapes, and surface properties [3, 4].

The proposed mechanism of plant-mediated AuNP synthesis involves the catalysis reduction of Au^{3+} ions through phytochemicals present in the plant extract. These phytochemicals simultaneously act as reducing and stabilizing agents, resulting in the formation of the monodisperse AuNPs. Techniques such as UV-visible spectroscopy, X-ray diffraction, and transmission electron microscopy were utilized for the characterization of the synthesized nanoparticles, elucidating their properties. TEM analysis indicated that spherical nano gold particles have around 10 nm in diameters. In this biosynthesis protocol, the gold nanoparticles with desired shape and size can be prepared.

These plant-mediated AuNPs can have numerous applications in diverse fields. In the biomedical sector, they demonstrate significant potential for drug delivery, imaging, and therapeutics. The unique properties of AuNPs, including their biocompatibility and surface plasmon resonance, enable targeted drug delivery and imaging, as well as efficient photothermal therapy. Additionally, the antimicrobial properties inherent in plant extracts can be leveraged in the development of antimicrobial films, coatings, and disinfectants incorporating AuNPs.

Keywords: Green catalyst; Gold Nanoparticles; Catalysis Reduction; Biosynthesis

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Cu(II) Complex of 3-Hydroxy-2-naphtoic acid (Cu-HNA) as an Efficient and Reusable Catalyst for the One Pot Synthesis of Naphthopyranopyrimidines Under Solvent-free Conditions

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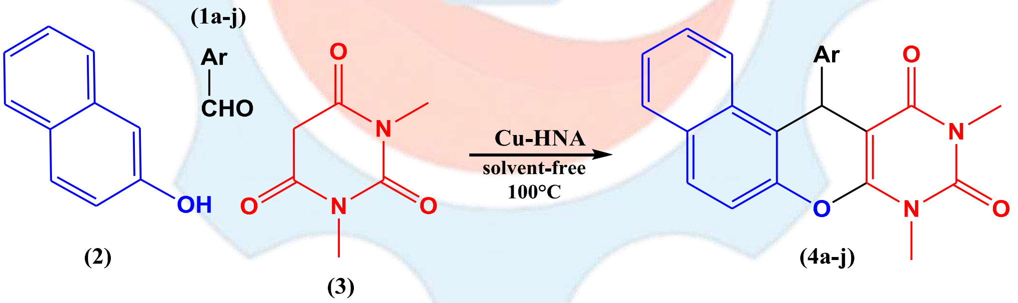
Pyrans belong to an important class of compounds which show a wide range of biological activities [1]. The pyranopyrimidines exhibit important biological properties such as anticancer, antitubercular activity, antifungal and antibacterial activities [2]. Naphthopyranopyrimidines are fused heterocyclic compounds that display antioxidant and antimicrobial activities [3]. Therefore, the development of simple methods for their synthesis is an important challenge. Undoubtedly, the synthesis of naphthopyranopyrimidines through multicomponent reactions (MCRs) of aldehydes, 2-naphthol and 1,3-dimethylbarbituric acid has been paid much attention due to excellent synthetic efficiency, inherent atom economy, procedural simplicity and environmental friendliness. Also, the possibility of performing multicomponent reactions under solvent-free conditions with a heterogeneous catalyst could improve their cost-effectiveness and ecological acceptability.

Because of the important role of transition metal complexes in coordination chemistry, especially in preparation of various catalysts [4], recently Mn^{+2} and Cu^{+2} complexes of 3-hydroxy-2-naphtoic acid have been synthesized [5].

Following of our systematic studies and researches on the expansion of practical, safe, and green procedures for synthesis of organic compounds using reusable solid acid catalysts [6], in this work, we illustrate an efficient method for the synthesis of of naphthopyranopyrimidines (**4a-j**) through condensation of aryl aldehydes (**1a-j**), 2-naphthol (**2**) and 1,3-dimethylbarbituric acid (**3**) using Cu-HNA as an effective heterogeneous catalyst at 100°C under solvent-free conditions (Scheme 1).

Keywords: 3-Hydroxy-2-naphtoic acid; Heterogeneous catalyst; Barbituric acid; Pyranopyrimidines; One-pot reaction; Solvent-free.



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An Overview of the use of Catalysts in Oil and Gas Industries

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With the growing trend of competition in production and achieving a quality final product in various industries, especially the oil and gas industry, scientists and researchers are looking for a way to reduce production time, increase product quality, cost price, and also reduce emissions. Are less Therefore, in the early 18th century, scientists proposed catalytic materials. These substances increase the rate of the reaction by reducing the activation energy level of the reaction without being consumed in the reaction. Also, one of the most important features that distinguishes these materials from other chemical materials is their recycling and regeneration [1], which, in addition to reducing environmental risks, also has an impact on time and costs. Catalysts play a key role in industries, especially petrochemical industries and refineries. In this industry, due to the different production units, such as sour naphtha desulfurization unit, cracking unit to increase efficiency, production of valuable synthetic materials, naphtha reforming unit to produce gasoline and isomerization, etc. [2] the need for catalysts that work in high operating conditions (temperature and high pressure) it is important not to lose their efficiency. For example, in the process of reforming naphtha to produce high-quality gasoline, due to the high operating temperature (750 degrees Celsius), if the right catalyst is not used, the catalyst is poisoned and its efficiency loses earlier than the scheduled time [3]. Due to the advancement of technology, Nano catalysts have occupied a special place due to their greater contact surface compared to other materials. So, in the treatment of industrial wastewater, the removal of harmful gases such as H_2S, Nano catalysts such as Nanographene, Nanorods, etc. [4] play a role. Do But despite the environmental limitations and the use of renewable resources, new catalysts have been made using solar cell technology, which has entered the field of competition with other catalysts as photocatalysts. Photocatalysts have a special place in many industries such as mineralization of organic pollutants, water and air purification, production of green fuel and preparation of organic compounds due to their low energy consumption and production costs, ease of carrying out reactions and their high performance at low temperature. A big step in the use of renewable resources [5].

Keywords: Catalyst; Selective Catalytic reduction; Naphtha; Nanotechnology; Renewable Energy

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PLA/CS-ZnO Nanocomposite for Rapid Catalytic Reduction of Nitrophenol Compounds as an Excellent Heterogeneous Nanocatalyst

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Abstract

In this research, a high efficiency and environmentally friendly method to reduce nitrophenol compounds such as 4-nitrophenol (4-NP), 2,4,6-trinitrophenol (2,4,6-TNP) and 2,4-dinitrophenol (2,4-DNP) was used in the presence of PLA/CS-ZnO nanocomposite. Using FT-IR, SEM, XRD and UV-Vis techniques, PLA/CS-ZnO nanocomposite was identified after synthesis. Also, the mechanical properties of the nanocomposite were investigated using the stress -strain curve. The mentioned nanocomposite showed a very good efficiency in reducing nitrophenol compounds to aminophenolic compounds, so that under optimal conditions, 100% conversion and selectivity in the reduction of 4-NP, 2,4,6-TNP and 2,4-DNP to 4-AP, 2,4,6-TAP and 2,4-DAP were observed. UV-Vis absorption spectrum at different times were used to evaluate the progress of the reaction. Furthermore, after the reaction, PLA/CS-ZnO was recovered and used for the next cycle. The results showed that the nanocomposite can perform ten consecutive cycles without a significant decrease in efficiency. The comparison of catalytic activity with other catalysts showed that the nanocomposite synthesized in the present research has a higher efficiency in reduction nitrophenol compounds.

Keywords: Nitrophenol Compounds, Chitosan, Reduction, Polylactic acid, Aminophenols.

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Determination of lorazepam and diazepam using modified nanocrystalline cellulose for ultrasonic-assisted dispersive solid-phase microextraction (UA-DSPME) and gas chromatography – mass spectrometry (GC-MS)

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Abstract

In this work, a quick and efficient method based on ultrasonic assisted-dispersive solid-phase microextraction coupled by gas chromatography/mass spectrometry (GC/MS) was developed for the determination of lorazepam and diazepam drugs from biological and aqueous samples. Effective sorbent based on modified nanocrystalline cellulose was simply prepared and applied for microextraction of the target analytes. The extraction efficiency of the different sorbents, such as the cellulose nanostructure and modified nanocrystalline cellulose by self-assembled N-(2-Aaminoethyl)-3-aminopropyltrimethoxysilane, were compared. The characterization of the modified cellulose nanostructure was performed using thermogravimetric analysis (TGA), energy dispersive X-ray (EDX), and fourier transform infrared spectroscopy (FTIR). In addition, the effects of different factors on extraction/desorption performance, such as extraction time, ionic strength, as well as the type and volume of desorption solvent were studied. The limits of detections (1 and 3 ng mL^{-1}) and quantifications (4 and 10 ng mL^{-1}) were obtained for lorazepam and diazepam, respectively. The developed method also showed good repeatability, relative standard deviation (RSD) 4% and 6% (n = 5), for the spiked aqueous solution at the concentration level of 50 ng mL^{-1} for analytes, and linearity, R>0.9996, in the range of 10-1000 ng mL^{-1}.

Keywords: Diazepam; Lorazepam; Ultrasonic-assisted dispersive solid phase microextraction (UA-DSPME); Gas chromatography/mass spectrometry (GC-MS); Biological samples; Modified cellulose nanostructure.

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Synthesis and investigation of catalytic activity of nanocellulose / nickel nanocomposite in the hydrolysis of sodium borohydride

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In this study, bacterial nanocellulose (BC) was utilized as an eco-friendly and biodegradable support to synthesize metal nanocomposites. Moreover, external reducing agents such as ascorbic acid, hydrazine hydrate, and sodium borohydride were used for the reduction of nickel salt. The nanocomposite (Ni/BC) was prepared by refluxing and drying in a vacuum oven. The structure of the nanocomposite was characterized using various techniques such as infrared spectroscopy (FT-IR), X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray energy dispersion measurement (EDS), and vibration magnetometer (VSM). The catalytic activity of Ni/BC was studied for the hydrolysis of sodium borohydride. The effect of various parameters such as catalyst content, sodium borohydride concentration, temperature, and pH were investigated. The nanocomposite exhibited excellent catalytic activity in the hydrolysis of sodium borohydride. According to the results, it was found that in neutral pH, ambient temperature, and optimum amount of catalyst, the hydrogen generation rate (HGR) was 160 mL min $^{-1}$g $^{-1}$ and the activation energy (Ea) was 32.17 kJ/mol. The study also revealed that nickel nanocomposite can be recovered in five steps, making it an economical sample.

Keywords: Nickel nanoparticles, nanocellulose, sodium borohydride, hydrolysis

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CO2 methanation using Ni catalysts supported on low-cost LTA-5A zeolite synthesized from pretreated Iranian coal gangue

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In this work, zeolite LTA-5A was synthesized for the first time from the coal gangue of Iranian mines and was used as a support for the preparation of nickel catalysts for the methanation of CO_2. These catalysts were characterized using XRD, FESEM, TEM, EDX, elemental mapping, H_2-TPR, CO_2-TPD, NH_3-TPD and low-temperature adsorption of Nitrogen. Different weight percentages of nickel metal were loaded on the desired zeolite support by the wet impregnation method (from 5 to 20%). The results showed that the prepared catalysts are different in terms of properties and catalytic efficiency (CO_2 conversion and CH_4 selectivity), which can be due to the difference in the size of the final nickel active sites caused by loading different amounts of nickel. In general, the performance of the catalysts examined in this research was close to and slightly lower than the catalysts prepared using commercial zeolites, but in any case, the results were promising for the use of hazardous coal gangue for the synthesis of value-added materials to reduce the amount of CO_2 emissions to the atmosphere.

Keywords: CO_2 methanation, LTA zeolite, coal gangue, Heterogeneous catalysis

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Visible- light active C,N-TiO2/LTA-4A zeolite photocatalyst preparation using coal gangue as Si and Al precursor

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Semiconductors play a pivotal role in photocatalysis, being photoexcited upon exposure to ultraviolet or visible light. ZnO, TiO_2, and WO_3 stand out as prominent semiconductors employed in this process. Notably, TiO_2 enjoys widespread utilization due to its advantageous attributes, including low toxicity, high chemical inertness, cost-effectiveness, and environmental friendliness. However, the intrinsic limitations of anatase TiO_2, such as its large bandgap energy of 3.2 eV exclusively active under UV light and rapid recombination of electron-hole pairs, necessitate strategic mitigation. An effective approach involves the incorporation or doping of metals (e.g., Ag and Pt) or non-metals (e.g., C and N) onto the TiO_2 nanoparticle surface. This modification aims to shift light absorption towards the visible light spectrum and extend the lifespan of charge carriers. Nevertheless, challenges persist, such as the potential reduction in photocatalytic efficiency due to nanoparticle aggregation and the impediments associated with the separation and recovery of these nanoparticles, leading to a significant increase in operational costs. To address these issues, the assembly of nanosized photocatalysts on porous supports, such as clays, zeolites, and carbon nanotubes, presents a viable solution. In this study, LTA-4A zeolite, successfully synthesized from coal gangue, serves as a catalyst support, onto which C,N-TiO_2 is doped as the active phase. The synthesized samples undergo comprehensive characterization through XRD, FESEM, EDX, UV-vis DRS, elemental mapping, and low-temperature N_2 adsorption analysis. This visible light-active photocatalyst exhibits promising potential for the removal of organic pollutants from water.

Keywords: photocatalysis, LTA zeolite, coal gangue, Heterogeneous catalysis, Visible-light

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Photoelectrocatalysis

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Abstract:

Photoelectrocatalysis, a synergistic integration of heterogeneous photocatalysis and electrocatalysis principles, encompasses a wide range of applications. These include the degradation of harmful compounds, the generation of H2 and O2 through water splitting, the reduction of nitrate, N2, and CO2, and the synthesis of valuable organic molecules. This innovative approach is particularly useful for producing compounds that are challenging to synthesize using traditional methods. Moreover, photoelectrocatalysis finds application in sensing and biosensing systems. The core of photoelectrocatalysis lies in leveraging the benefits of the heterogeneous photocatalytic process by applying a biased potential to a photoelectrode supporting the catalyst. This configuration enhances the separation efficiency of photogenerated charges. By applying a biased potential, the photoelectrode ensures that the energy from light irradiation exceeds the band gap energy of the semiconductor. Consequently, this leads to an extended lifetime of electron-hole pairs. The recent advancements in photoelectrocatalysis are closely tied to the evolution of materials, with a particular emphasis on 2D and nano materials. Highly ordered nanomaterials like graphene, nanotubes, and nanowires are gaining prominence due to their large surface area and excellent conductivity. Overcoming challenges involves developing stable semiconductor materials capable of activation through solar radiation. In essence, the method relies on a semiconductor that is irradiated by light energy equal to or greater than its band gap energy, while simultaneously being biased by a gradient potential. Therefore, a comprehensive understanding of photoelectrocatalytic processes necessitates a grasp of both the fundamental aspects of photocatalysis and electrocatalysis. The objective of this lecture is to bridge this gap by delving into the essential principles and scope of photoelectrocatalysis.

Synthesis and characterization of the CoNi-MOF as an electrocatalyst for the CO_2 reduction reaction (CO_2RR)

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The electrochemical reduction of carbon dioxide (CO_2) has been widely utilized as a method for converting CO_2 into valuable chemical fuel. One of the significant products obtained from CO_2 reduction is formate (HCO^{-2}). However, the conversion of CO2 into hydrocarbon, formate, has faced significant energy barriers. In this study, we have achieved a remarkable breakthrough by successfully achieving a highly efficient electrochemical conversion of CO_2 to formate using a CoNi-MOF catalyst. we have achieved a substantially reduced onset potential for formate production, as low as -0.4 volts versus the reversible hydrogen electrode (RHE). Moreover, the CoNi-MOF showed a stable CO_2 electroreduction capability for up to 30 h. The high performance of CoNi-MOF for CO_2 electroreduction was ascribed to the rod morphology as well as the presence of Co and Mn species.

The increased current density on CoNi-MOF facilitates the enhanced rate of CO_2 reduction. We believe that the findings of this study will not only advance the development of MOF-catalysts for CO_2 conversion but also deepen our understanding of the effects of these electrocatalysts on CO_2 reduction. Finally, we report the CoNi-MOF electrocatalyst that achieves an excellent current density of 75.5 mA/cm^2 at −1.1 V vs RHE.

Keywords: Catalysts, Electrochemical Reduction, CO_2 Reduction, Redox Reactions

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Effective use of domestically synthesized catalyst to produce polyvinyl chloride with high efficiency

Meysam Souri

Polyvinyl chloride (PVC) is one of the most important polymers. Population growth and industrialization of countries have multiplied the need for this valuable material.

The synthesis of this important substance in the presence of the Ethyl Hydroxy Piperazine (EHP) catalyst in liquid form will increase productivity to a very high extent. Considering the sanctions and economic issues of domestic production of this catalyst, it can increase productivity and reduce reaction time. In addition, the PVC product produced has a high percentage of purity.

In the present research work, the EHP catalyst was synthesized on a laboratory scale with much higher quality and higher efficiency. The synthesized catalyst was used to produce PVC with 100% efficiency.

Keyword: Polyvinyl chloride, Ethyl Hydroxy Piperazine, catalyst

Nitrogen-doped graphyne nanosheet for CO_2 reduction reaction: A DFT calculation

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To protect the environment and reduce greenhouse gases, adsorption, isolation, and reduction of CO_2 are from the most important scientific challenges [1]. Nowadays, research on two-dimensional nanomaterials for CO_2 adsorption and reduction is increasing [2]. Graphyne (GY) is a carbon nanostructure contains carbon atoms with sp and sp^2 hybridization, which uses as catalyst for doing this reaction due to its high surface-to-volume ratio [3]. In this research, we have conducted a theoretical study on graphyne doped with a nitrogen atom (GY-N) as a substrate for reducing CO_2 to formic acid (HCOOH). In the following, the adsorption rate of CO_2 and H_2 on the pure and N-doped graphyne was compared and investigated. All of our calculations were performed using Grimm's modified density functional method (DFT-D) at the GGA-PBE level of theory and the DNP basis set with the help of the DMol3 module in the Materials Studio software. The results showed that the cohesive energy of the N atom on the graphyne sheet is equal to -6.977 eV. The highest adsorption energy of CO_2 molecule on the pure and N-doped graphyne structures is related to the horizontal direction at site H1, with adsorption energies of -0.185 and -0.177 eV respectively. Also, the highest adsorption energy of the H_2 molecule on these structures is related to the vertical and oblique directions respectively at site H1, with adsorption energies of -0.117 and -0.116 eV, respectively. Next, the mechanism of reduction of CO_2 on the substrate N-GY was investigated. According to the obtained results, in the first and second stages, gases CO_2 and H_2 are consumed separately as reactants. In the third step, hydrogen connected to nitrogen is connected to the formate molecule, and the final product of HCOOH with a stable energy of -0.46 eV is produced. The rate-determining step in this path has an energy barrier of 2.27 eV, which is related to the first step of the reaction. Our findings show that the obtained product is thermodynamically and kinetically favorable. So using N atom doping on the graphyne structure can be effective in designing a suitable catalyst for the reduction of CO_2.

Keywords: Graphyne; Carbon nanostructures; DFT; CO_2 reduction; Doping.

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Computational study of the carbon dioxide hydrogenation to formic acid on to Ni,N/graphyne

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In the recent years, unique properties and characteristics of the carbon nanostructures have led to a lot of research in the field of science and nanotechnology. Graphyne is a flat sheet of carbon atoms that was first proposed in 1957 by Baughman et al [1-2]. The presence of acetylenic groups and flexibility in the structure of graphyne have caused this material to show interesting applications in the field of sensors, transistors, purifiers, and catalysts. Todays, one of the concerns related to global warming is the increase of the greenhouse gases such as CO_2, which is known as the main cause of the global warming. Therefore, it is necessary to find methods to reduce or eliminate CO_2 in the atmosphere [3]. In the present work, with the help of H_2 gas, we investigated the CO_2 adsorption ability and the reduction reaction of CO_2 on graphyne substrate that simultaneously decorated and doped with Ni and N atoms, respectively. Our theoretical calculations were performed using the modified Grimm density functional method (DFT-D) at the GGA-PBE level of theory and the DNP basis set with the help of the DMol3 module in the Materials Studio software. After optimization, in the most stable state CO_2 molecule can be horizontally adsorbed on the substrate Ni-GY-N at site H1 with energy -0.200 eV. Also, the highest adsorption energy of H_2 gas on this substrate is at position H1, in the horizontal direction with a value of -0.752 eV. Next, to check the catalytic properties of Ni-GY-N substrate, H_2 gas is optimized horizontally as a reactant on the structure in the first step. Then the activation energy for H_2 dissociation determined that is equal to 1.90 eV, and hydrogen atoms are separated from each other and join to N and Ni atoms. In the second step, the CO_2 molecule is horizontally added to the structure as the second reactant. After optimization, the hydrogen atom attached to the nickel atom is joined to the carbon atom of the CO_2 molecule. The activation energy of this step is equal to 1.44 eV. In the third step, the formate molecule on the Ni-GY-N-H substrate is considered. The activation energy of this step is equal to 0.50 eV and by creating O-H bond, formic acid is produced as the final product. Our findings show that this mechanism, having the activation energy of 1.90 eV in the first step, is favorable from the point of view of kinetics and thermodynamics, and the structure of Ni-GY-N is suggested as a suitable catalyst for CO_2 reduction.

Keywords: Graphyne; DFT; Carbon nanostructures; Decoration; CO_2 hydrogenation.

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CO_2 methanation using Ni catalysts supported on low-cost LTA-5A zeolite synthesized from pretreated Iranian coal gangue

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In this work, ZnO-CuO/Kaolinite nanocomposite with different molar ratios of Zn to Cu was prepared and used to remove *Staphylococcus aureus* and *Escherichia coli* bacteria from water. The response surface method was used to evaluate the efficiency of the prepared nanocomposites in the photocatalytic removal of the desired bacteria under ultraviolet and visible radiation. Factors affecting the photocatalytic process were studied, including the photocatalyst dose, Zn to Cu molar ratio in the nanocomposite, the exposure time, and the type of radiation source. The results showed that the optimal value in the molar ratio of Zn to Cu is equal to 8:1. Optimal levels of other factors under visible light are photocatalyst dosage of 20 $mg.ml^{-1}$ and 120 minutes of exposure time. The optimal photocatalyst dosage and contact time levels under ultraviolet radiation are 50 $mg.ml^{-1}$ to 80 $mg.ml^{-1}$ and 20 minutes.

Keywords: Photocatalytic decomposition, Nanocomposite materials, Visible-light, Ultraviolet light

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Synthesis of [2-amino-3-(ethoxycarbonyl)-1,4- dihydro-1-phenyl-4-pyridinyl] ferrocene and their theoretical studies

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The literature has documented the four-component reaction involving amines, acetylenic esters, aromatic aldehydes, and ethyl cyanoacetate, which leads to the synthesis of 1,4-dihydropyridine derivatives under various conditions [1]. Numerous methods and catalysts have been employed for the synthesis of 1,4-dihydropyridines, including Sm/ZrO2, Et_3N and etc [2]. These methods involve the use of microwaves, ionic liquids, and reflux at high temperatures. 1,4-Dihydropyridines belong to a class of compounds that exhibit various biological activities, such as antiviral, antioxidant, anti-tumor, anti-inflammatory, antimicrobial, antitubercular, antihistaminic, and anticancer activities [3]. In line with our interest in the synthesis of ferrocene compounds, we report the synthesis of [2-amino-3-(ethoxycarbonyl)-1,4-dihydro-1-phenyl-4-pyridinyl]ferrocene derivatives through a four-component reaction involving ferrocenecarboxaldehyde **(1)**, ethyl cyanoacetate **(2)**, aniline **(3)**, and acetylenic esters **(4)** in the presence of 20 % mol piperidine. This reaction yields high yields and occurs under mild reaction conditions. For theoretical investigations, we substituted the substituents of 1,4-dihydropyridine with hydrogen atoms and explored the electronic parameters, vibrations, and hyperpolarizability of [1,4-dihydro-1-phenyl-4-pyridinyl]ferrocene.

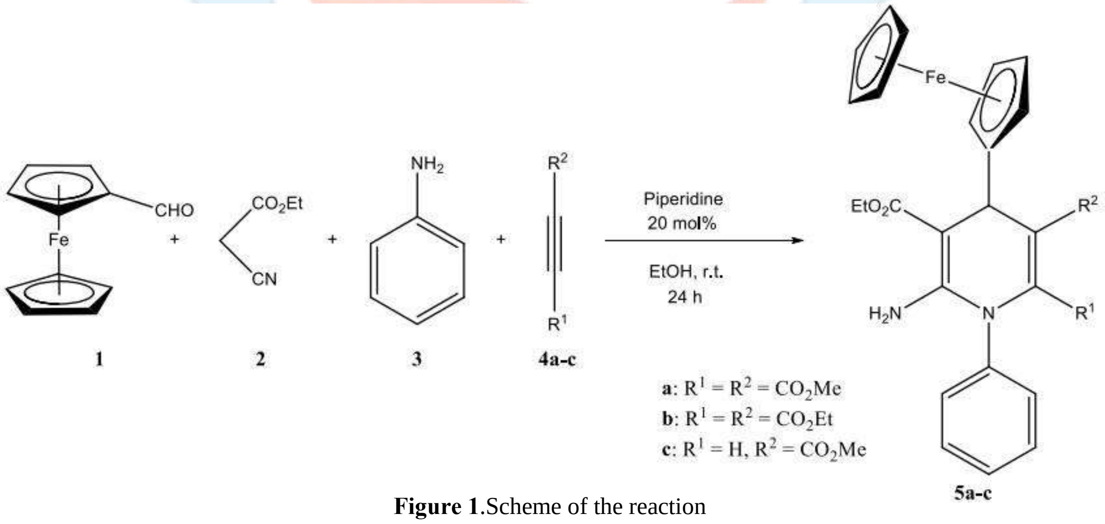

Figure 1.Scheme of the reaction

Keywords: Ethyl cyanoacetate; 1,4-dihydropyridine; acetylenic esters; piperidine

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Ternary Heterojunction Engineering through Construction of $NiCo_2O_4$@MOF-801@MIL88A Photocatalyst for Degradation of Inorganic and Organic Pollutants

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This research developed a new photocatalyst called $NiCo_2O_4$@MOF-801@MIL88A through a simple and cost-effective process and utilized it as a photocatalyst for water treatment applications. The novel nanocomposite was characterized using several analytical techniques such as XRD, IR, XPS, TEM, SEM, TGA, BET, EIS, PL, and UV–vis. Through analysis, it was discovered that the heterojunction structure formed between the components enhanced the photocatalytic performance by preventing the recombination of charge carriers. Photocatalytic simulation tests were also performed to demonstrate the material's effectiveness in reducing chromium and degrading antibiotics. The composite demonstrated better performance than pure components or $NiCo_2O_4$@MOF-801 under visible light illumination for Cr(IV) reduction and antibiotic (Meropenem) degradation. The various factors such as drug concentrations, reaction pH, photocatalyst amount, scavenger type, etc., were investigated to optimize the reactions and improve photocatalytic response. The addition of MIL-88A and changing the bandgap improved the photocatalytic reactions and reduced the time needed. In particular, the main photocatalyst, $NiCo_2O_4$@MOF-801@MIL88A, reduced 100% of Cr(IV) in just 45 minutes, indicating significantly improved photocatalytic activity due to interface connection and charge-carrier separation. Overall, the study provides valuable insights into the development of sustainable energies for water treatment applications. Nanomaterials as photocatalysts offer promising solutions to the global energy crisis, and the synthesized material shows potential for removing both organic and inorganic contaminants from the water source [1, 2].

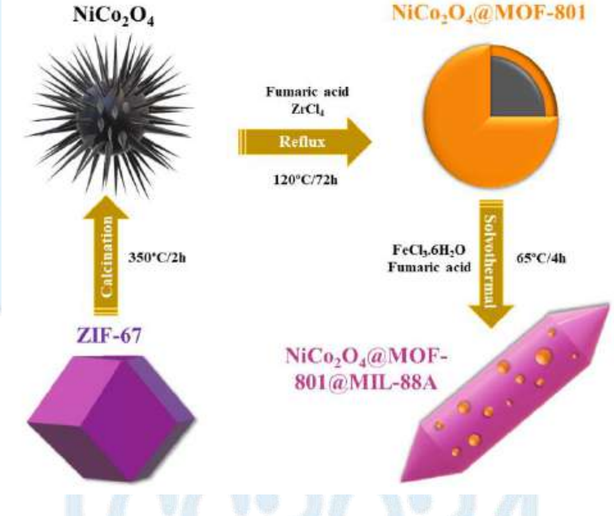

Figure 1. The synthesis process of $NiCo_2O_4$@MOF-801@MIL-88A heterojunction.

Keywords: Photocatalyst; Water treatment; MOF-on-MOF; Heterostructures;

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Polyvinylidene Fluoride Film Loaded with Ce-based MetalOrganic Framework for Efficient Reduction of Cr(VI) from Wastewater

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Abstract:

The development of efficient and recyclable water treatment technologies is critical for the practical removal of Cr(VI) from wastewater. Ce-based metal-organic frameworks (Ce-MOFs) are widely used in water treatment due to their high surface area, water stability, and multiple active sites[1]. However, the use of powdery Ce-MOFs presents several challenges, including difficulty in reclamation, secondary pollution, and aggregation. To overcome these issues, we successfully loaded Ce-MOF onto a polyvinylidene fluoride (PVDF) film using the phase inversion method[2], resulting in a highly efficient photocatalyst for the adsorption and photoreduction of Cr(VI)[3]. The prepared photocatalyst demonstrated the ability to reduce 70% of chromium solution for 120 minutes under visible light. XRD and UV-vis analysis confirmed the formation of a heterojunction structure between the components, which prevented charge carrier recombination and improved photocatalytic performance. Overall, our study presents a cost-effective material with high efficiency for removing inorganic contaminants from water.

Keywords: metal-organic frameworks, PVDF, chromium (VI)

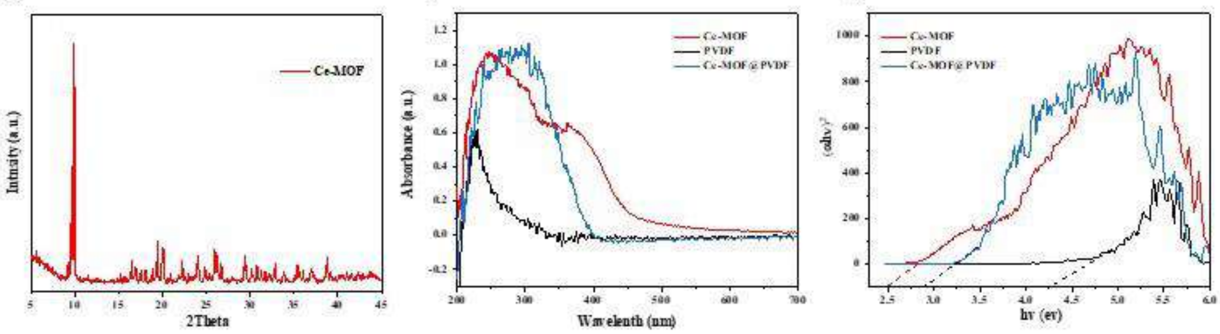

Figure 1. (a) Powder XRD pattern, (b) UV−vis DRS spectra (c) corresponding Tauc plots.

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Defective frameworks Based on MOFs for Efficient Photocatalytic NO Abatement

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Abstract

The design of accurately directional electron transfer channels at the interface of catalysts is still considered a huge challenge. In this pathway, efficient photoactive constructions derived from novel MOFs were employed as promising models to precisely build the atomic-level interface electrons transfer channels via carbon-metal bonding. An optimized composite framework with plasmonic species and oxygen vacancies exhibited an improved photocatalytic removal efficiency for the ppb-level atmospheric NO, which is interestingly higher than that of the pristine inorganic materials. The enhanced photocatalytic performance is owing to appropriately-constructed electron transport channels with loaded graphitic carbon as a bridge in our system. Further theoretical calculations can be performed to demonstrate the built-in graphitic carbon-metal bridges and as-related effects which justify the Schottky barrier between the pure inorganic component and (probable) metal nanoparticles in the framework, enhancing the photoelectron transfer efficiency. Such works represent exciting cases for the modulation of photoelectron transfer at the catalysts interface for air purification.

Keywords: MOF, NO abatement, Photocatalyst, Defects

Fast and efficient catalytic degradation of methyl orange via UiO-66 based membrane

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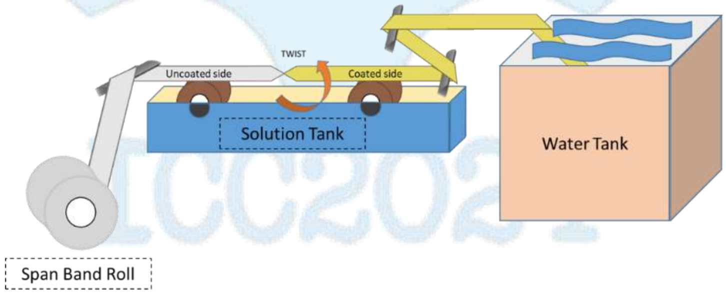
Advancements in the utilization of Metal-Organic Frameworks (MOFs) in specific domains frequently face challenges due to the recovery and stability issues. For example, the catalytic elimination of aqueous pollutants from water often leads to the leaching and loss of the catalyst. Numerous strategies have been developed to mitigate this problem. Granulation and coating are of the most effective methods for anchoring nanoparticles on the substrate surface to avoid leaching and losing materials. The latter method, coating, garners significant interest due to the precise control, ease of synthesis procedure and the potential for further functionalization. In this study, we have successfully devised a method, phase inversion roll coating process to synthesize a uniformly thin membrane for the catalytic removal of the anionic dye, methyl orange in water.

A comprehensive structural analysis, encompassing techniques such as Powder X-ray Diffraction (PXRD), Fourier Transform Infrared Spectroscopy (FT-IR), Brunauer–Emmett–Teller (BET) theory, Scanning Electron Microscopy (SEM), etc., was conducted on the synthesized MOF and membrane to confirm the successful coating of the adsorbent on the surface of polystyrene fibers. Subsequently, the membrane was employed to catalytically remove methyl orange from water, and various adsorption and degradation parameters were examined. Finally, an appropriate mechanism and adsorption capacity of the materials were proposed.



Keywords: Metal-Organic Framework, DMMP, Catalyst, UiO-66

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Oxygen Evolution Reaction (OER) Promoted by Co(III) Carboxamide Complexes

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Water splitting stands out as an efficient method for generating high-purity hydrogen and oxygen [1]. Notably, significant advancements have been achieved in the development of molecular catalysts for oxygen production, employing earth-abundant transition metals. Cobalt complexes featuring polypyridyl ligands, known for their stability and electroactivity at both metal and ligand centers, have garnered considerable attention [2]. Within this context, a Co(III) complexes, with the formula of [CoL (X)(OH_2)], where L = N,N bis (pyridine-2-carboxamido) benzene dianion and X= Br and I, has been synthesized and meticulously characterized using CHN elemental analysis, IR, UV-Vis, and X-ray powder diffraction techniques.

The crystal structure analysis of the complexes reveals that the dianionic ligand L, forming an N4 set, is situated in the equatorial plane. Simultaneously, the two H_2O and X ligands occupy the axial positions, resulting in a distorted octahedral geometry around the Co(III) center [3]. The electrocatalytic performance of these complexes in water splitting reactions has been explored, demonstrating commendable electrocatalytic activity in the oxygen evolution reaction with a good turnover frequency at pH=8.

Our methodology for synthesizing effective and stable molecular catalysts with earth-abundant transition metal ions presents a straightforward approach to design and fabricate molecular electrocatalysts for the oxygen evolution reaction (OER) process.

Keywords: Water Splitting; Carboxamide; Co(III) Complexes; Oxygen Evolution Reaction (OER)

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Synthesis of dihydropyrano[2,3-c]pyrazole derivatives using superparamagnetic nanocatalyst Fe_3O_4@gly@Furfural@Co$(NO_3)_2$ in green conditions

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Pyrano [*2, 3-c*] pyrazoles are scaffolds that have received much attention from chemists due to their use in various fields such as pharmaceuticals, agriculture, and industries. Pyrano pyrazoles act as an analgesic, anticancer, antifungal, vasodilator, and antimicrobial. [1-3] In recent times, environmental concerns have led chemists to devote their efforts to developing methods that are environmentally friendly. Extensive research has been done in this field. Among the different branches of green chemistry, the design of catalysts that are both non-toxic and recyclable is of great importance. Currently, the use of magnetic nanoparticles (MNPs) in the synthesis of organic compounds has been widely considered due to the ease of separation of MNPs from the reaction solution using an external magnet. As a result, there is no need to rely on difficult separation techniques such as centrifugation or filtration. [4,5]. Here, we introduced a cheap and accessible method for the synthesis of pyrano[*2,3*-c]pyrazole compounds from the reaction between ethyl acetoacetate, hydrazine hydrate, aryl aldehyde and malononitrile using Fe_3O_4@gly@Furfural@Co$(NO_3)_2$ MNPs, and this method has advantages such as the use of green solvents, non-toxicity and relatively high efficiency, and nanocatalyst can be recycled up to 5 steps (scheme1) .

Scheme 1. Synthesis of substituted dihydropyrano[2,3-c]pyrazole by Fe_3O_4@gly@Furfural@Co$(NO_3)_2$

Keywords: Magnetic nanoparticles; Pyarano[*2,3*-c]pyrazple; Green conditions; Cobalt (п) nitrate.

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Synthesis of Polyhydroquinolines using superparamagnetic nanocatalyst Fe_3O_4@gly@Furfural@$Co(NO_3)_2$

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Multi-component reactions (MCRs) have garnered significant interest for their utility in synthesizing intricate and varied compounds with biological properties, offering rapid synthesis without the need for purification and isolation of intermediates, resulting in reduced waste, high yields, simultaneous reactions of multiple substances, low energy consumption, and excellent selectivity [1].Polyhydroquinoline derivatives, as a different category of heterocyclic compounds, exhibit efficacy in addressing cardiovascular disease and possessing anti-tumor, anti-tuberculosis, anti-bacterial, and antimalarial properties [2]. In recent years, nanomaterials have found numerous applications in various fields such as biology, chemistry, pharmaceuticals, and medicine, with Fe_3O_4 magnetic nanoparticles exhibiting superior properties including high catalytic performance, high surface-to-volume ratio, easy synthesis, high thermal and mechanical stability, and reusability [3]. In summary, a new and straightforward method for producing polyhydroquinoline derivatives has been introduced through the reaction of ethyl acetoacetate, dimedone, ammonium acetate, and aromatic aldehydes at 80°C using Fe_3O_4@gly@Furfural@$Co(NO_3)_2$ as a reusable catalyst, offering advantages such as a simple work-up procedure, the use of inexpensive and readily available starting materials, a short reaction time, the use of a safe and recyclable nanocatalyst, a wide range of substrates, solvent-free reactions, and high to excellent yields (Scheme 1).

Keywords: Polyhydroquinoline; Magnetic nanocatalyst; Multicomponent reaction.

Schem 1: Synthesis of Polyhydroquinoline by Fe_3O_4@gly@Furfural@$CO(NO_3)_2$

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$[Mo_{176}]$-GO Nanofiber-based Solid Phase Extraction Procedure Coupled with HPLC Analysis for the Quantification of Zolpidem in Human Urine Samples

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In this work, a solid phase extraction (SPE) method based on nanofibers was applied to the extraction and purification of zolpidem from urine samples. A clean-up cartridge was homemade and polystyrene nanofibers were spun and selected as the adsorption material. After the SPE procedure, the obtained extraction solution was analyzed by high performance liquid chromatography (HPLC). The nanofibers type, adsorbent amount and desorption conditions were the main factors affecting the extraction efficiency and were optimized in detail. Under the optimal conditions, good linearity was obtained in the range of 1-12 µg/mL with the correlation coefficients (r) above 0.99. The LOD of the analyte was 0.3-0.5 µg/mL, and the LOQ were 0.5-1.1 µg/mL. The intra- and inter-day precision (RSD) values of this method were within the acceptable ranges of 1.35-15.7% and 3.8-15.2%, respectively. The recovery determined for the zolpidem at the three concentration levels were in the range of 91.3-115.4%. These results showed that the home-made cartridge has an excellent extraction efficiency for the studied compounds. Compared to other common pretreatment method, the proposed method is simple and reliable.

Keywords: Extraction, Nanofiber, Zolpidem, Graphene Oxide.

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Nanoball-MWCNT for the Solid Phase Extraction of Methadone as Nanofiber Film

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Multiwalled carbon nanotubes (MWCNTs) were synthesized with $Mo_{72}Fe_{30}$ nanoparticles (MWCNTs-$Mo_{72}Fe_{30}$-NPs) and subsequently electrospining by polyacrylonitrile (PAN). The hollow-fiber was used for the microextraction of the methadone from urine and wastewater samples under the optimized conditions as sensitive technique to determinate methadone.

In many countries of the world, the selected treatment for opiates dependence is methadone maintenance therapy (MMT). Methadone, also known as Methadose, Dolophine, Amidone, Symoron, Physeptone, Heptadon and many other names, is a synthetic analgesic drug which is commonly used to treat dependence on heroin and other opioids since the mid-1960s.

After optimizing the reaction conditions, extraction of methadone in the presence of hollow-fiber combined with fluorescence spectrophotometry was performed. The MWCNTs-$Mo_{72}Fe_{30}$ composite has many practical advantages over the reported nanomaterials modified electrodes for the detection of methadone, such as cost-effective, highly reproducible and can be prepared in short period of time.

Central composite design under response surface methodology was used for the evaluation of the effect of variables, individually, as well as their possible interaction effects on the adsorption process. The relative standard deviation for the analyte was found to be lower than 2.14%. The MWCNT- $Mo_{72}Fe_{30}$-NPs nanofiber film adsorption capacity was found to be 41.07mgg^{-1}. The enrichment and preconcentration factors were found to be 107.01 and 98.21, respectively. The developed method was finally applied successfully to the determination of methadone in urine and wastewater samples with the recoveries ranged from 95.32 to 104.1%.

Keywords: Microextraction, Nanofiber, Methadone, Carbon nanotube.

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Highly Active and Stable COF Based on Plasma Treatment Serve as Effective Photocatalyst for the Desulfurization of Dibenzothiophene under Visible Light Irradiation

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In the large attempts to seek technologies exploiting sustainable sources of energy, photocatalysis as a robust and fascinating technology consolidate its privileged position among other different potentialities for evolution in visible light-driven organic reactions in an environmentally green and sustainable manner. In this point of view, LED that is broadly reachable and cost-effective set to be a desired alternative for light resources, such as solar, mercury, UV, etc.

Covalent organic frameworks (COFs) have been situated in the spotlight of scientific attention as a supporting material for photocatalyst incorporation due to their notable specific surface area providing effective distribution for photocatalyst, additionally, existence of functional groups would furnishes COFs with binding sites assisting the photocatalytic activity improvement.

In this context, we motivated to present an ingenious, novel and facile prospect for synthesizing nitrogen-rich covalent organic framework (N_2@COF) by plasma technique and used as a photocatalyst under blue LED irradiation. As a matter of fact, plasma through the deploying pure gas of N_2 without requiring toxic precursors and organic solvents or waste stream, making the employed process in this work remarkably green and sustainable. On the other hand, plasma is a contributing factor in decreasing band gap energy related to N_2@COF comparison with pure COF.

An outstanding research interest has grown concerning the selective photocatalytic oxidation of organic compounds owing to the earning expansive of chemical reactions in a sustainable and green approach. Deep oxidative desulfurization (ODS) of dibenzothiophene is one of the most appealing chemical transformations, which brings a remarkably observable effect on earning various essential organic compounds in both biological as well as industrial areas. The real value of the organic transformation techniques becomes more vivid when a whole package of green chemistry rules merges into one path to gain phenomenal efficiencies as opposed to the lowest detrimental consequences on the environment. According to this objective, plasma treatment equip this work with a green medium as an eco-friendly factor, simultaneously acting in line with the improvement of the performance of photooxidation reactions.

The sophisticated role of plasma-treatment on the photocatalytic activity improvement is by no means negligible. The band gap energies of COF and N_2@COF are 2.8 eV and 2.3 eV, respectively. It is evident that a considerable decrease on band gap energy and red shift take place by employing plasma technique. The selective photocatalytic desulfurization of dibenzothiophene to corresponding sulfone was successfully performed by applying N_2@COF in the existence of sustainable and green oxidant of H_2O_2 after 3 h emission of four high blue LED 3 W lamp at room temperature. Key factors that lead to nominate plasma, N_2@COF and LED irradiation are the requirements of designing sustainable systems to gain green chemistry targets. This environmentally friendly strategy has illustrated numerous merits such as operational facileness, cost-effective, high efficiency of photocatalyst, non-toxic nature, utilizing blue LED as visible light source, time-saving, and mild reaction conditions. Additionally, N_2@COF is recyclable after executing at least five reaction cycles without any drop in photocatalytic performance, which can meet the sustainable process index.

Keywords: COF; Plasma; Photocatalyst; Desulfurization; Blue LED

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PVC/TiO_2 membrane for Photocatalytic removal of malachite green

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Pollution of water resources is one of the biggest challenges facing human society and dyes are among the main contaminants of water resources [1]. Malachite green is a cationic dye that is used as dye in leather and textile industries, and due to the anti-fungal properties of this color, it is widely used in agriculture and fish breeding industries [2]. Several methods have been proposed to remove the malachite green color in the environment, among which photocatalytic degradation has received much attention due to the possibility of reusing the used catalysts and producing mineral products with less toxicity. Titanium dioxide is considered an efficient catalyst for the photocatalytic degradation of pollutants due to the rapid transfer of electrons to molecular oxygen [3].

In the present study a polymeric membrane containing polyvinyl chloride (PVC) as the base polymer, titanium dioxide (TiO_2) as the photocatalyst, and dioctyl phthalate (DOP) as a plasticizer were fabricated, characterized by scanning electron microscope (SEM), energy-dispersive X-ray spectroscopy (EDS) and fourier transform infrared spectroscopy (FT-IR), and used for the photocatalytic removal of malachite green from aqueous solution, this membrane showed 59% removal in two hour for a concentration of 5 ppm of the dye under UV light. This shows good efficiency of catalyst for photocatalytic degradation of malachite green.

Keywords: Malachite green, TiO_2, photocatalytic degradation

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Synthesis and characterization of bimetallic metal-organic frameworks based on Zr and Cd for absorption and photocatalytic degradation of organophosphorus compounds

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Metal organic frameworks (MOFs) have been widely investigated as adsorbents and catalysts to remove pollutants in wastewater [1]. The UiO-66 is one of the representative MOFs that demonstrates excellent chemical, mechanical and thermal stability [2]. Herein bimetallic zirconium-cadmium MOF (Zr/Cd-MOF) is synthesized by hydrothermal method and its photocatalytic performance to degrade organophosphorus compounds under visible light were explored in detail. The result of Mott– Schottky tests certified the formation of n–n heterojunction between Cd-MOF and UiO-66, which is conducive to the transfer and separation of photogenerated electrons and holes and is the main reason of the enhanced photocatalytic performance [3]. The photocatalyst was characterized by using several physicochemical methods such as Fourier transform infrared (FT-IR), Diffuse-reflectance spectra (DRS), X-ray diffraction (XRD), Scanning electron microscopy (SEM), Energy dispersive X-ray spectroscopy (EDS) mapping analysis, and Transmission electron microscope (TEM). In addition, the mechanism of photocatalytic degradation of Cd/Zr-MOF was studied by adding different eliminating agents. The photodegradation of organophosphorus compounds was mainly caused by superoxide ion ($^{\cdot}O^{2-}$) and electron hole (h^+).

Keywords: metal organic framework; bimetallic MOF; photocatalyst; photocatalytic degradation; organophosphorus compounds

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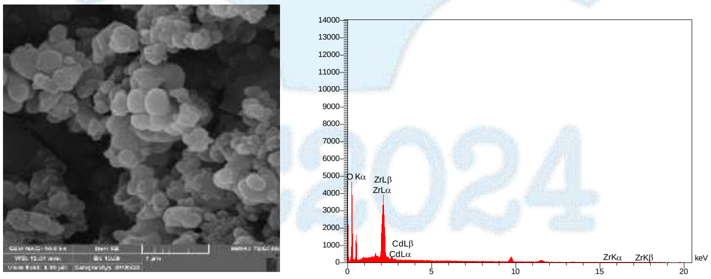

Fig. 1. SEM and EDX of Cd/Zr-MOF prepared by hydrothermal method.

Synthesis and characterization of bimetallic metal-organic frameworks based on Zr and Cd and composite it with g-C_3N_5 for absorption and photocatalytic degradation of organophosphorus compounds

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Metal–organic frameworks (MOFs) are a new group of molecular networks arranged in a three-dimensional skeleton with metal centers and bridged organic ligands around them [1]. The MOFs have a remarkable performance in the fields of adsorption [2], separation [3], photocatalysis [4], and drug delivery [5]. On the other hand the adsorption and photocatalytic degradation of hazardous materials such as organophosphorus compounds by adsorbents with high adsorption capacities and easy separation from sample solutions are highly desirable. In this research, the photocatalytic degradation of organophosphorus compounds in real specimens was developed using an bimetallic metal-organic framework composite with the addition of g-C_3N_5 as an adsorbent. The adsorption of organophosphorus compounds on Cd/Zr-MOF/g-C_3N_5 was optimized by considering various factors including pH, amount of adsorbent, contact time and sample concentration. Results with scavengers allowed concluding that $O_2^{\bullet -}$ radicals are the main reactive species, although photogenerated $^{\bullet}$OH radicals and electrons also contribute to the degradation.

Keywords: bimetallic MOF; MOF/g-C_3N_5; photocatalyst; photocatalytic degradation; organophosphorus compounds

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Synthesis and characterization of bimetallic metal-organic frameworks based on Cu and Zr for absorption and photocatalytic degradation of organophosphorus compounds

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Metal-organic framework (MOF) is a new class of porous crystalline materials featured with regular pores, open channels and high surface area [1,2]. In particular, a few bimetallic MOFs can be obtained when two kinds of metal ions are coordinated with ligands among the MOF structures [3]. Adsorption desulfurization is very effective for the removal of organophosphorus compounds from the environment. The metal-organic frameworks have emerged as a new type of adsorbents because of their porous nature and large specific surface area [4]. In this study, Cu^{2+} was covalently introduced into the UiO-66 framework at the defective sites with H_2BDC as a ligand by the solvothermal method. Then, the structure of the synthesized compounds is investigated by using Scanning electron microscopy (SEM), Transmission electron microscope (TEM), Energy dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), Diffuse-reflectance spectra (DRS) and Fourier transform infrared (FT-IR). The photocatalytic activities were investigated via the degradation of organophosphorus pesticides using the Cu/Zr MOFs under UV light irradiation. On the basis of the results, a possible photocatalytic mechanism of the prepared samples was proposed. The results indicate that Cu/Zr bimetallic metal-organic framework have great application potential in pollutant degradation.

Keywords: metal organic framework; bimetallic MOF; photocatalyst; photocatalytic degradation; organophosphorus compounds

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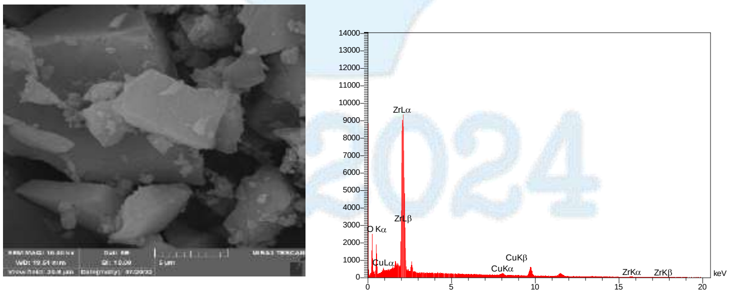

Fig. 1. SEM and EDX of Cu/Zr-MOF prepared by hydrothermal method.

Novel fatty alkanolamide synthesis from date seed oil as biodegradable feedstock using heterogeneous catalyst

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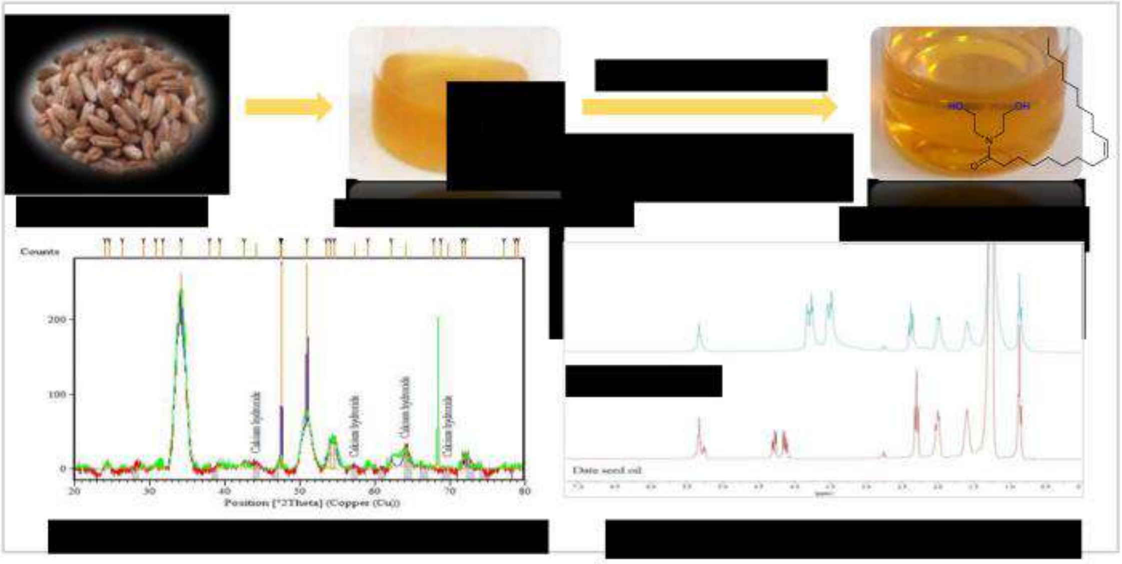
In this study, we aimed to directly convert date seed oil into fatty alkanolamide through a one-step, solvent-free amidation process. To achieve this, we utilized a heterogeneous catalyst, Na/Ca$(OH)_2$, which was prepared using a simple wet chemical method. The catalyst was characterized using FT-IR and powder XRD. Complete conversion (   ) of date seed oil to alkanolamide has been obtained in just 1 hour and, respectively, using 10 mol% Na/Ca $(OH)_2$ as the heterogeneous catalyst and a 3:1 molar ratio of diethanolamine:date seed oil at 110°C. This catalyst was equally effective for the amidation reaction of date seed oil. Amidation is a reaction that involves the reaction between a vegetable oil or fatty acid and an amine compounds, such as diethanolamine. Typically, homogeneous catalysts are used for synthesizing fatty acid alkyl amides. Previous researches has utilized acidic or basic, and/or metal-modified zeolites as catalysts. The formation of amide bonds in natural products and bioactive molecules has the potential to significantly alter their chemical, physical, and biological properties. These amide bonds are also the basis for many drug molecules and polymers synthesis. Alkanolamides have a wide range of applications, including foam-control agents, lubricants, surfactants, fungicides, water repellents, shampoos, detergents, and antiblocking agents in plastics processing technologies[1]. One advantage of using natural triglycerides as a feedstock is their availability. Additionally, these vegetable oilbased materials are environmentally safe, biodegradable, and non-toxic sources [2].



Scheme: DSO alkanolamide synthesis by Na/Ca $(OH)_2$ heterogeneous catalyst

Keywords: heterogeneous catalyst, date seed oil (DSO), fatty alkaolamide, Amidation

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In-situ epoxidation of Date seed oil as bio-renewable feedstock with mineral acid homogeneous catalyst

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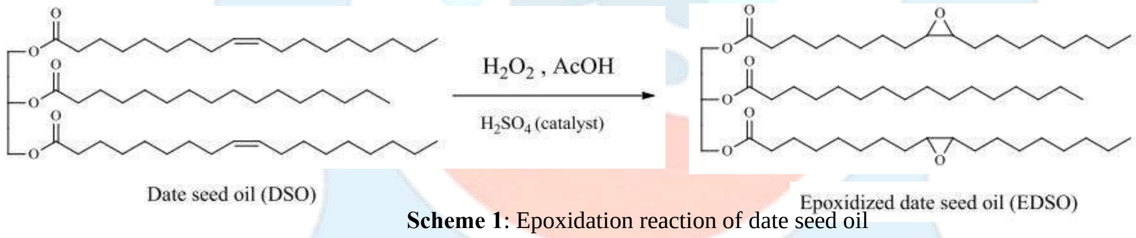
In recent times, environmental concerns such as the depletion of petroleum sources, global warming, and widespread pollution have been continuously worsening [1]. As a result, vegetable oil (VO) has become a crucial bio-resource due to its affordability, easy availability, and environmental restoration properties. VOs are mixtures of triglycerides, which consist of three fatty acid chains connected by a glycerol backbone. These fatty acid chains are mostly unsaturated, with zero to three double bonds per chain. The epoxidation reaction involves the reaction between the double bond of carbon-carbon in the fatty acid chains and active oxygen, resulting in the formation of an oxirane ring [2]. Epoxidated vegetable oils (EVOs) are widely used in various industrial applications, such as plasticizers, and are mainly used in the production of synthesized polyols or polyesters, glycol, carbonyl compounds, and bio-lubricants [3]. The date (Phoenix dactylifera L.) is a crucial product in the social and economic life of people in arid and semi-arid regions of the world, providing nourishment and contributing to economic growth [4]. Date seeds are a by-product of date products such as date syrup, date juice, date powders, pitted dates, and date confectionery [5]. In this study, a novel EVO was obtained from date seed oil (DSO). The epoxidation of DSO was carried out using sulfuric acid as a mineral acid homogeneous catalyst, in combination with H_2O_2 as the oxidant and AcOH as an additive (**Scheme 1**). The epoxidized date seed oil was successfully achieved under mild conditions, and the main functional groups were identified using FT-IR and ^{1}HNMR spectroscopy.

Keywords: Epoxidation, Date seed oil (DSO), epoxidized date seed oil (EDSO), homogeneous catalyst



Scheme 1: Epoxidation reaction of date seed oil

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QM study on inhibition mechanism of carbonic anhydrase enzyme as a bio catalyst by phenolic inhibitors

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Carbonic anhydrase metalo-enzyme is a bio catalyst which is acts as PH regulator and metabolic enzyme in all forms of life that catalyzes the reversible hydration of carbon dioxide to bicarbonate and a proton, eq. 1 and 2.

$$[EZn^{2+}(OH^{-})]^{+} + CO_2 \leftrightarrow [EZn^{2+}(HCO_3^{-})]^{+} \leftrightarrow [EZn^{2+}(OH_2)]^{+} + HCO_3^{-} \qquad (1)$$

$$[EZn^{2+}(OH_2)]^{+} \leftrightarrow [EZn^{2+}(OH^{-}) + H^{+} \qquad (2)$$

The zinc ion, Zn (II) in carbonic anhydrase bio catalyst is critical for the inhibition path of this enzyme. So, designing agents that interfere with CA catalytic mechanism in order to obtain pharmacological agents with a novel action mechanism is one of the most important fields of research in recent years. Besides, some different inhibition mechanisms have been proposed for CA isoenzymes. Carbonic anhydrase inhibitors (CAIs) usually were divided to two classical and non-classical groups. In the classical CAIs, Inhibitors molecule coordinate directly to the metal at the center of active site and from tetrahedral, trigonal or bi-pyramidal geometries. Sulfonamides and their thioesters and metal chelating anions are the most classical studied inhibitors. Besides, Phenolic compounds are one the most important of inhibitors which indirect interaction with zinc ion in the centre of the active site [1, 2]. In the present research the inhibition mechanism of human carbonic anhydrase isoform II, hCAII, with some phenolic compounds, which are distributed in plant tissues as a secondary metabolite, including phenol, catechol, resorcinol, 4-methyl catechol, vanillic acid, trans-cinnamic acid and *ortho*-coumaric acid was investigated using quantum mechanical calculations. According to quantum mechanical calculated results all phenolic inhibitors do not directly interact with the zinc ion in the CA active site and just interact with oxygen atom which coordinated to zinc ion, Figure 1.

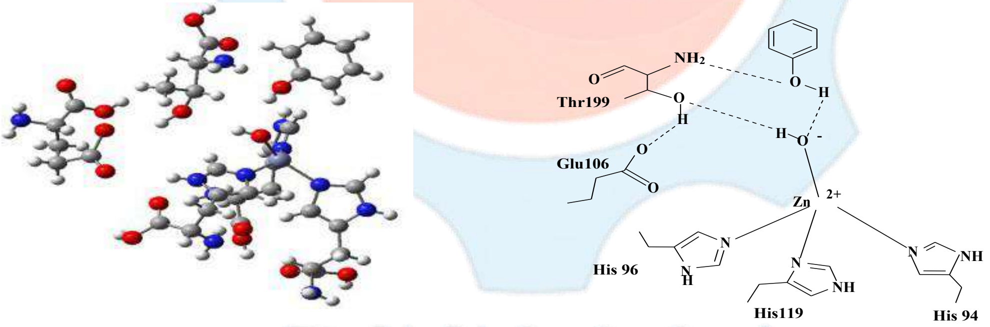

Figure 1. Interaction of phenol with the active site of carbonic anhydrase bio catalyst

Keywords: Carbonic anhydrase; Phenolic compound; Inhibitor; DFT calculations

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Comparative Analysis of Fe-Mn Catalyst and Bimetallic Catalysts for Light Olefin Production via Fischer-Tropsch Synthesis

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The Fischer-Tropsch process is the cornerstone of the conversion of synthesis gas into a wide range of hydrocarbons, with a particular focus on the production of light olefins, which serve as key precursors in the petrochemical industry. Due to the importance of bimetallic catalysts in the Fischer-Tropsch process, they offer the possibility of fine-tuning the catalytic properties to meet the needs of a specific product and increase the overall efficiency of the process. In the present work, a Fe-Mn bimetallic catalyst was prepared by the impregnation method. The catalyst was characterized by XRD, BET, and FE-SEM methods. The catalytic activity was evaluated in a fixed-bed reactor at a pressure of 1.0 MPa, $H2/CO = 1$, and GHSV = 10 L h^{-1} g_{cat}^{-1} in the temperature range of 300-360 °C. The effect of temperature and the second active metal on the performance of the catalyst was then investigated. CO conversion and product selectivity were also calculated from the GC results. The results showed that higher temperatures increased the selectivity of light olefins by a higher percentage. In order to evaluate the performance of the Fe-Mn catalyst as a suitable catalyst for light olefin production, the results of the present work were compared with Fe-Sn and Fe-Cu bimetallic catalysts from other articles in terms of light olefin selectivity and CO conversion. The paper concludes with an outline of future perspectives and research directions. This emphasizes the importance of selecting the right catalyst to optimize light olefin production and points to future developments in Fischer-Tropsch synthesis.

Keywords: Fischer-Tropsch process, Light olefin, Fe-Mn catalyst, Bimetallic catalysts, Petrochemical industry

Rational Design of Ti_3C_2 MXene Nanocomposite with Bromophenol blue for efficient signal amplification: Sensitive Electrochemical Detection of Cardiac Troponin I in Patient Plasma

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Despite considerable prognostic advancements over the last decade, acute myocardial infarction (AMI) remains a leading cause of morbidity and mortality globally [1]. Myocardial damage is irreversible, with 85% of cardiac damage occurring within two hours of a heart attack, and delaying medical treatment increases the risk of death [2]. As a result, the development of an affordable, sensitive, accurate, and timely AMI diagnosis, is critical for improving survival rates. Toward this end, targeting suitable biomarkers is highly desirable [3] . Today, although a new generation of two-dimensional (2D) MXenes has received considerable interest throughout several fields, the rational design of MXene-based nanocomposites and their particular applications in biosensors remain serious challenges. Herein, to avoid etched-loosely accumulated accordion-like structure of Ti_3C_2 MXene to restacking, delamination was conducted using bromophenol blue (BPB), which makes the resulting BPB@Ti_3C_2 nanocomposite as an ideal nanolable for ultrasensitive detection of acute myocardial infarction (AMI) biomarker (cardiac troponin I, cTnI). For this purpose, after sandwiching the cTnI between covalently-bonded Tro4 aptamer on the BPB@Ti_3C_2 and MNPs/Tro6, the electrocatalytic activity of the nanolabel towards H_2O_2 was followed as a tracer signal. Owing to i) high effective surface area for immobilization of the Tro4 and ii) large electrocatalytic activity of the BPB@Ti_3C_2 for electroreduction of H_2O_2, along with iii) enrichment characteristic of the MNPs/Tro6, as well as iv) the synergistic-assisted signal amplification between the Ti_3C_2 and BPB, high sensitive detection of cTnI has been introduced. The developed biofunctionalized BPB@Ti_3C_2 exhibits a wide dynamic range of 200 fg mL^{-1}-250 ng mL^{-1} with a low detection limit of 20 fg mL^{-1}. The aptasandwich form was used to quantify the cTnI in the human blood plasma of cardiovascular patients, above 90% clinical sensitivity, providing a promising strategy for clinical diagnosis and biochemistry research.

Keywords: Cardiac troponin I, Aptasensor, Electrochemical, Ti_3C_2 MXene, Hydrogen peroxide, Nanocomposite.

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Photocatalytic performance of a magnetic nanocomposite containing Cu(BDC) for dye removal

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This research reports the synthesis of bismuth ferrite nanoparticles and metal-organic framework, Cu(BDC), by applying microwaveassisted combustion in solid state and ultrasound-assisted method, respectively. The characteristics of both materials were improved by forming them into a composite through ultrasonic probe strategies. This approach increased the photocatalytic property of bismuth ferrite nanoparticles and created the magnetic property of the metal-organic framework. Various analyses, such as FT-IR, XRD, SEM and UV-Vis were used to verify the accuracy of the synthesis. The catalytic performances of the nanoparticles and the nanocomposites were evaluated by examining their photocatalytic degradation of dye. The results demonstrated that the nanocomposite developed in this study can be a potential candidate for eliminating contaminants from wastewater. The properties of bismuth ferrite, Cu(BDC) and $BiFeO_3$/Cu(BDC) nanocomposite were studied thoroughly.

Keywords: Photocatalytic degradation, Metal organic framework, Magnetic nanocomposite, Degradation of dye.

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Synthesis of Polycaprolactone/TiO2 Composite 3D Membrane for Photocatalytic Degradation of Methylene Blue

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Abstract:

The contamination of waterways by industrial dyes constitutes a significant environmental concern, with methylene blue being a common pollutant. This has necessitated the development of efficient and sustainable methods for the treatment of dye-laden waste water [1].

This study introduces a novel photocatalytic foam composed of polycaprolactone (PCL) and titanium dioxide (TiO_2) as an efficacious solution for the degradation of methylene blue [2]. The synthesis of PCL/TiO_2 foam involves the dispersal of TiO_2 nanoparticles within a PCL matrix, creating a composite with a high surface-area-to-volume ratio, which is advantageous for photocatalytic reactions. The photocatalytic performance of the composite foam was evaluated under UV light irradiation, with experiments demonstrating substantial elimination of methylene blue. Various parameters such as the initial dye concentration, foam dosage, pH levels, and irradiation time were optimized to achieve maximal degradation efficiency. Furthermore, the reusability and stability of the PCL/TiO_2 foam were examined over multiple cycles of photodegradation, indicating the material's potential as a reusable photocatalyst for wastewater treatment applications. With this research, 67% destruction was observed.

The study proposes that the PCL/TiO2 foam is a promising, low-cost, and effective material for the photocatalytic treatment of methylene blue in contaminated water, meriting further exploration for the remediation of a variety of organic pollutants.

Keywords: 3D membrane, Photocatalytic, Polycaprolactone

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ZIF-68 MetalOrganic Framework is an effective catalyst for preparing 2-amino-4H chromenes using ultrasonic irradiation

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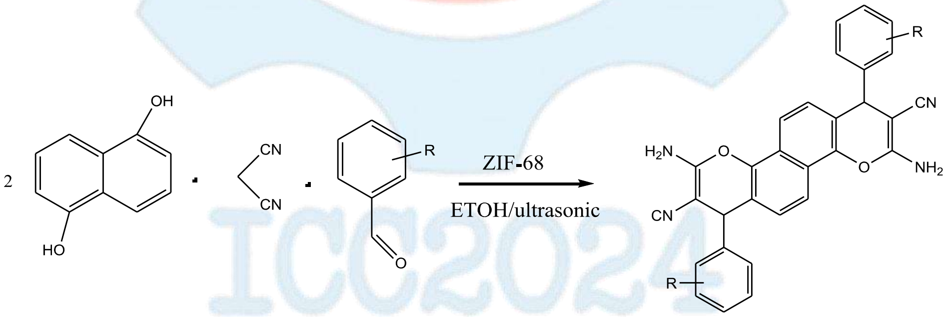
One of the progressive strategies which have recently attracted considerable attention is the usage of ultrasound conditions with heterogeneous catalysts. 2-Amino-4H chromenes are an important class for further development in medicinal and organic synthesis studies due to their potency and a wide spectrum of biological activities including cancer therapy, antiviral, antitumor and sex hormone. The preparation of 2-Amino-4H-Chromenes has been reported using various conditions and catalysts. Most of the reported methods require long reaction times, the use of toxic solvents, low yields, non-reusable catalysts, and stoichiometric reagents. Te synthesis of substances under ultrasonic condition not only requires fewer catalysts and solvents, but also meets the environmental requirements more powerfully [1-2]. In this study, ZIF-68 MetalOrganic Framework was applied as a magnetically and robust catalyst to prepared the bicyclic 2-amino-4H-chromenes (**Scheme 1**) [3].



Scheme 1: Preparation of 2-amino-4H-chromenes derivatives

Keywords: MetalOrganic Framework, ZIF-68, 2-Amino-4H chromenes

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Enhancement of Nickel Recovery from Spent DRI Catalyst using H_2SO_4 containing Cl^- ions solution followed by Ni^{+2} ions Cementation by Aluminum powder

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The extraction and recovery methods of metals offer a proficient and sustainable method for recovering valuable metals from waste generated by industrial catalysts, thereby mitigating the hazards linked to their disposal. This work presents a novel two-step method that combines hydrometallurgical and electrochemical techniques to examine the extraction and retrieval of nickel from spent direct reduction of iron (DRI) catalysts. During the extraction process, the leaching system employs a combination of H_2SO_4 and NaCl. In the subsequent purification stage, metallic powder is acquired by reducing Ni^{+2} ions with the aid of Al powder. In order to evaluate the impact of chlorine ions on the selectivity and extraction conditions of nickel from alumina support, a statistical analysis is conducted using the design of experiments (DOE) technique. This procedure was used to systematically evaluate crucial factors, including temperature (20-80°C), duration (60-200 min), H_2SO_4 concentration (2-4M), and NaCl amount (0-0.16 g/ml). By utilizing the Box-Behnken Design (BBD), two quadratic models were created, both of which achieved an R^2 value over 96%. These models effectively combine important variables, quadratic relations, and binary interactions, enabling accurate forecasts for the extraction of nickel and aluminum. Under conditions of low temperatures and high concentrations of sulfuric acid, the presence of chlorine ions has a more noticeable impact, resulting in greater selectivity and considerably improved efficiency in the leaching process. Through the utilization of numerical optimization techniques, it was determined that the most favorable parameters for the process were a 73°C, 160.5 min, 3M H_2SO_4, and 0.16g/ml NaCl. Under these circumstances, the leaching process resulted in the complete extraction of nickel (100%) and a minor amount of aluminum (1.39%). These conditions were obtained at a pulp density of 0.1g/ml and a particle size below 150µm. The cementation process utilizing Al powder encountered difficulties that impacted both the efficacy and the purity of the nickel powder. The key parameters for overcoming these constraints were determined to be temperature and starting pH (pH_0). The recovery process yielded a Ni^{+2} ion recovery rate over 98%, resulting in magnetic Ni powder with a purity exceeding 99%. The experiment was conducted under optimal circumstances, with a pH_0 of 0.4, a temperature of 80 ºC, and an Al/Ni ratio of 6 (stoichiometric ratio). The quality of nickel powder was evaluated using ICP, SEM, and EDX analysis.

Keywords: Hydrometallurgical process; Spent DRI Catalyst; DOE approach; Cementation; Magnetic Ni powder;

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Efficient Platinum Recovery from Spent Reforming Catalysts: A Combined Hydrometallurgy and Activated Carbon Adsorption Approach

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The extraction and purification of platinum from industrial catalyst waste represent a sophisticated and eco-friendly approach to repurposing this valuable metal. This practice not only mitigates environmental impacts but also reduces the economic losses stemming from the improper disposal of depleted platinum catalysts. Our study introduces a bespoke two-step process, integrating hydrometallurgical and adsorption methods, for the efficient recovery of platinum from spent reforming catalysts. Initially, the leaching phase employs an HCl/HNO_3 system, followed by a purification stage where a high-purity platinum solution is obtained via the selective adsorption of $PtCl6^{2-}$ ions on activated carbon. To analyze the influence of crucial parameters and extraction conditions on platinum extraction from catalyst bases, a statistical investigation is conducted using the design of experiments (DOE) approach. During this phase, crucial parameters were methodically investigated, including temperature (25-85°C), time (30-180 min), solution to solid ratio (5-15 ml/g), and the stoichiometric ratio of HNO_3/HCl (1-7). Through the application of the Box-Behnken Design (BBD), the quadratic model has been formulated with an impressive R^2 exceeding 98%. This model incorporates essential parameters, quadratic relations, and binary interactions, providing a robust framework for accurate predictions in %Pt extraction. Through the use of numerical optimization techniques, it was determined that the leaching process achieved a full extraction of Pt when conducted at the optimum conditions of 81°C, 77 min, 14 ml/g solution to solid ratio, and 9 times the stoichiometric ratio of HNO_3/HCl. In the subsequent phase of the study, we evaluated the recovery of liquid-phase platinum using surface absorption with active carbon (AC). Initial tests were conducted to investigate variations in temperature, time and solution initial pH, with the goal of determining AC's absorption capacity for Pt. The analysis of the data indicated that AC exhibited a 92% absorption rate of Pt within duration of 6.3 h at a pH level of 2 and at ambient temperature. Furthermore, the absorption of other contaminants, such as aluminum ions, was low.

Keywords: Platinum; Spent reforming catalysts; Hydrometallurgical; Adsorption; Design Of Experiments (DOE)

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Design and synthesis of heterogeneous photocatalysts based on copper

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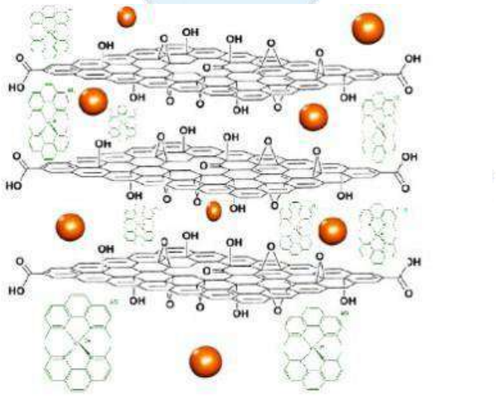
In recent years, the use of photocatalysts to perform oxidation-reduction reactions using light energy (as a renewable and endless source) to perform chemical reactions has attracted special attention; Because the transformation of low-value organic substances into valuable structures has always been one of the great attractions in chemistry. The International Union of Pure and Applied Chemistry (IUPAC) defines photocatalysis as "photocatalysis function as a change in the rate of a chemical reaction or its initiation under the action of ultraviolet, visible, or infrared radiation in the presence of a substance, the photocatalyst, that absorbs light and is involved in the chemical transformation of the reaction partners, or simpler terms, reactions that are carried out in the presence of semiconductors and light [1]. The use of copper-based catalysts has several advantages, such as abundant oxidation states (Cu(0), Cu(I), Cu(II), Cu(III)), non-toxic and adjustable, which can activate various functional groups through oxidation and reduction reactions [2]. The tendency of adjustable oxidation states of copper(I-III) species through the single electron transfer (SET) mechanism in the presence of an oxidant makes it a suitable candidate for the oxidation or dehydrogenation of organic molecules [3-4]. In this study, we prepared graphene oxide @ Fe_3O_4 nanoparticles modified with $Cu(II)dmp_2Cl_2$ (dmp=2,9-dimethyl-1,l0-phenanthroline) complex, resulting in the formation of a reusable heterogeneous photocatalyst (Scheme 1). $GO@Fe_3O_4@Cu(II)dmp_2Cl_2$ exhibited enhanced activity in catalyzing single electron transfer (SET) reactions between maleimide and tertiary aniline derivatives. To the best of our knowledge, there is no published study related to the synthesis of new derivatives of 5-methyl-2-phenyl 3a,4,5,9b-tetrahydro-1H-pyrrolo (3,4-c) quinoline-1,3 (2H)-dione using $GO@Fe_3O_4@Cu(II)dmp_2Cl_2$ photocatalyst. The synthesized photocatalyst has been identified by FT-IR, FE-SEM, and XRD analyses, and all the synthesized derivatives were characterized by spectroscopy methods.



Scheme 1: General scheme of $GO@Fe_3O_4@Cu(II)dmp_2Cl_2$ catalyst

Keywords: Photocatalyst, single electron transfer reaction, visible light

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Copper-supported on functionalized nano NaY zeolite with arginine and its application in synthesis of heterocyclic compounds such as pyrans

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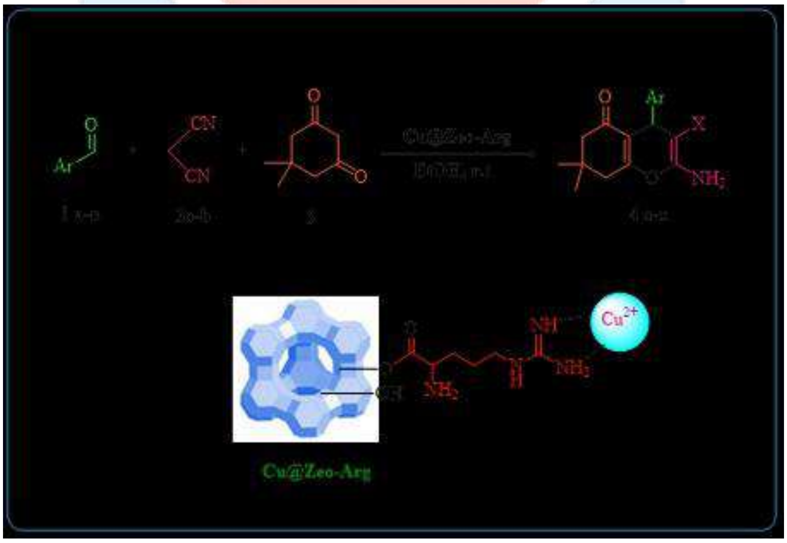
Today, the use of catalysts to reduce biological pollution and chemical waste has become very important and common. Meanwhile, heterogeneous catalysts are more widely used due to their special advantages such as recyclability, easy separation, and corrosion prevention. However, these catalysts suffer from some disadvantages such as low activity, low dispersion, and homogeneity. The homogenization of heterogeneous catalysts, including the attachment of different organic groups to the catalyst substrate, can improve the activity, efficiency, and homogenization properties of the catalyst [1-5].

As heterogeneous catalysts, zeolites have attracted much attention due to their unique properties such as stability, non-toxicity, availability, high porosity and high surface area [6-10]. On the other hand, amino acids have been widely used as an organic ligand in the functionalization of solid surfaces due to their unique structural features. Among them, arginine (Arg) is a natural, non-toxic, available and biologically active amino acid [11,12].

In this work, a new heterogeneous nanocatalyst, Cu@Zeo-Arg, was prepared by functionalizing NaY nanozeolite with amino acid arginine and then immobilizing copper metal on its surface. The formation of these nanocatalysts has been fully investigated and confirmed by various analyzes such as IR, TGA, CHN, BET, SEM, XRD, DLS, ICP and EDS Mapping. Considering the unique biological and chemical properties of 2-amino-4H-pyran and their wide application in industry, the activity of Cu@Zeo-Arg nanocatalyst was investigated in the synthesis of 2-amino-4H-pyran derivatives. 2-Amino-4H-pyrans were synthesized in good to high yields (72-95%) in the presence of Cu@Zeo-Arg catalyst in ethanol at room temperature within 1 h. The prepared nanocatalyst has special advantages such as easy preparation, high stability, high efficiency, mild conditions and short time, and the ability to recycle the catalyst in seven consecutive steps without a noticeable decrease in activity. The structure of the obtained products was identified and confirmed by measuring the melting point and data obtained from their 1H NMR, 13C NMR and IR spectra.

Keywords: Nanocatalysts; Heterogeneous catalysts; NaY nano zeolite; Arginine; Copper acetate; Pyran



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Numerical analysis of graphene plasmonics nanocatalyst and its application in energy harvesting

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Graphene plasmonics nanocatalyst is an emerging field at the intersection of graphene, plasmonics, and catalysis. Graphene, a two-dimensional carbon material with exceptional properties. Plasmonics, on the other hand, deals with the manipulation of light at the nanoscale, specifically the interaction between light and collective electron oscillations known as plasmons. By combining graphene with plasmonics, researchers have opened up exciting opportunities in catalysis. The unique properties of graphene, such as its high surface area, excellent electrical conductivity, and mechanical strength, make it an ideal platform for various catalytic reactions. Graphene plasmonics nanocatalysts have shown enhanced performance in several catalytic reactions, including hydrogen evolution, oxygen reduction, and various organic transformations. Plasmon resonance in metallic nanoparticles or graphene can enhance light-matter interactions, leading to improved catalytic activity and selectivity. The localized surface plasmon resonance (LSPR) phenomenon can enhance light harvesting, facilitate charge transfer, and generate hot carriers, all of which can promote catalytic reactions. Moreover, plasmon-driven catalysis can also be tuned by controlling the excitation wavelength, plasmonic materials, and catalyst-graphene interfaces. Research in graphene plasmonics nanocatalysts is still in its early stages, but promising results have been obtained so far. However, challenges regarding scalability, stability, and precise control over catalytic reactions still need to be addressed. Nevertheless, the integration of graphene, plasmonics, and catalysis holds tremendous potential for advancing various fields such as energy conversion, environmental remediation, and chemical synthesis. Here, with numerical simulation an absorption in graphene plasmonics nanocatalyst is inspected as shown in Fig.1.

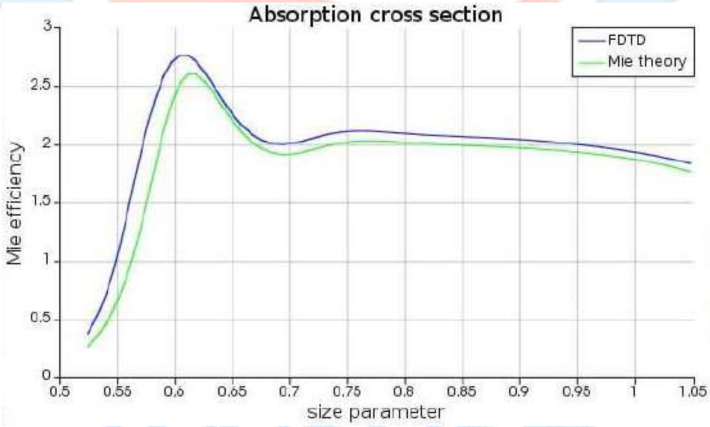

Fig. 1. Simulation of graphene plasmonics nanocatalyst

From Fig.1, graphene nanocatalysts have gained significant attention in the field of energy harvesting due to their remarkable properties including strong light-matter interaction, high conductivity, remarkable stability, and low-cost synthesis possibilities. Furthermore, graphene's versatility allows for functionalization and tuning of its properties, enabling the design of customized catalysts for specific energy harvesting applications.

Finally, graphene-based nanocatalysts combined with plasmonic structures can accelerate the process of water splitting, a critical step in hydrogen production. Plasmonic effects facilitate the harvesting of solar energy and enhance the photocatalytic activity of graphene, leading to efficient hydrogen generation.

Keywords: Graphene; Nanocatalyst; Plasmonics

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Innovative Synthesis of manganese oxide Nanoparticles from Cressa Leaf Extract for the Preparation of Catalytic Melem@Mn3O4 -HPA

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Abstract

Multi-component condensation reactions are essential for the synthesis of a wide range of organic compounds, including biologically active molecules [1]. Medicinal heterocyclic derivatives are significant chemicals that can be synthesized through various synthetic routes or isolated from natural sources. Bicyclic indoles have attracted attention due to their potential in drug discovery. Substituted indoles are known for their strong binding ability to high-affinity receptors and diverse physiological activities, including antimicrobial, anti-inflammatory, antimalarial, analgesic, anticancer, and antioxidant properties. Indoles also exhibit potential cytotoxic activities against various diseases, such as liver cancer, leukemia, diabetes, and hypertension [2-3] Metal oxides are chemical compounds resulting from the bonding of a metal with oxygen. They are prevalent in nature as minerals and play a pivotal role in various industrial processes. With diverse properties and applications, metal oxides serve as pigments in paints, essential components in the production of ceramics and glass, and catalysts in chemical reactions and environmental remediation processes. Their multifaceted significance makes metal oxides an indispensable class of compounds in both natural and industrial contexts [4]. The development of sustainable and environmentally friendly catalytic systems relies on improving catalyst efficiency, isolated yield, product selectivity, and reducing energy consumption. manganese oxide nanoparticles have been introduced as efficient catalysts in the chemical synthesis of a wide range of valuable organic compounds, including condensed indole derivatives, aromatic heterocycles, substituted tetrazoles, quinolines, and polyhydroquinolines. This highlights their potential as catalysts in the advancement of sustainable chemical processes [5].

The newly developed catalyst, Melem@Mn_3O_4-HPA, was synthesized by combining manganese oxide with melem and $H_5PW_{10}V_2O_{40}$. The resulting nanomaterial's structure was was confirmed using FESEM, EDS, XRD, and FTIR. This catalyst was then employed for the synthesis of 2-substituted indoles. This process provided a convenient method to obtain various 2- substituted (Indole) (phenyl) methylmalononitriles with potential biological activities. The reactions were performed in mild conditions such as low temperature and short reaction time with desirable yields. Optimization of reaction conditions is of critical case for successful synthesis. Solvent, temperature, time and amount of catalyst were studied. Substituted (indole) (phenyl) methylmalononitrile was synthesized in the presence of the heterogeneous catalytic system Melem@Mn_3O_4-HPA (0.03 g) from the relevant substrates under solvent-free conditions at 50 °C for 60 minutes with high efficiency. This experiment indicated that Melem@Mn_3O_4-HPA performed significantly better than other catalysts, resulting in a 95% yield at that time. The results demonstrated that Melem@Mn_3O_4-HPA is a highly efficient catalyst for the desired condensation reaction and exhibited excellent recyclability for at least five runs without significant loss of activity.Moreover, it has been established that the formation of 2-substituted indoles occurs through a radical mechanism, with •O2$^-$, h+, and OH• as contributing species. Additionally, the hot-filtration experiment confirmed that Melem@Mn_3O_4-HPA is a stable nanocatalyst in the current multicomponent synthesis.

Keywords: heterogeneous catalysis ; aromatic aldehydes; Mn_3O_4; 2-substituted indoles

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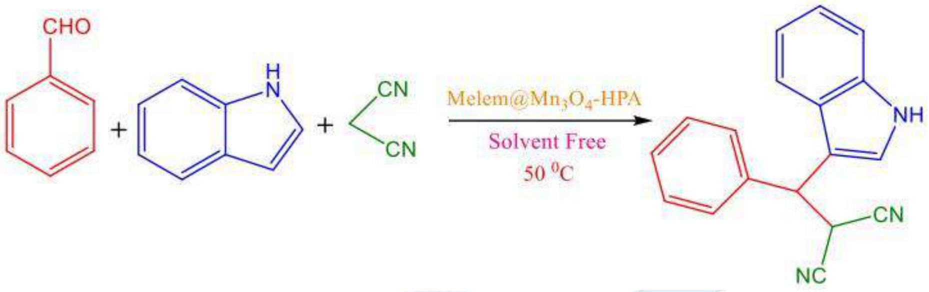

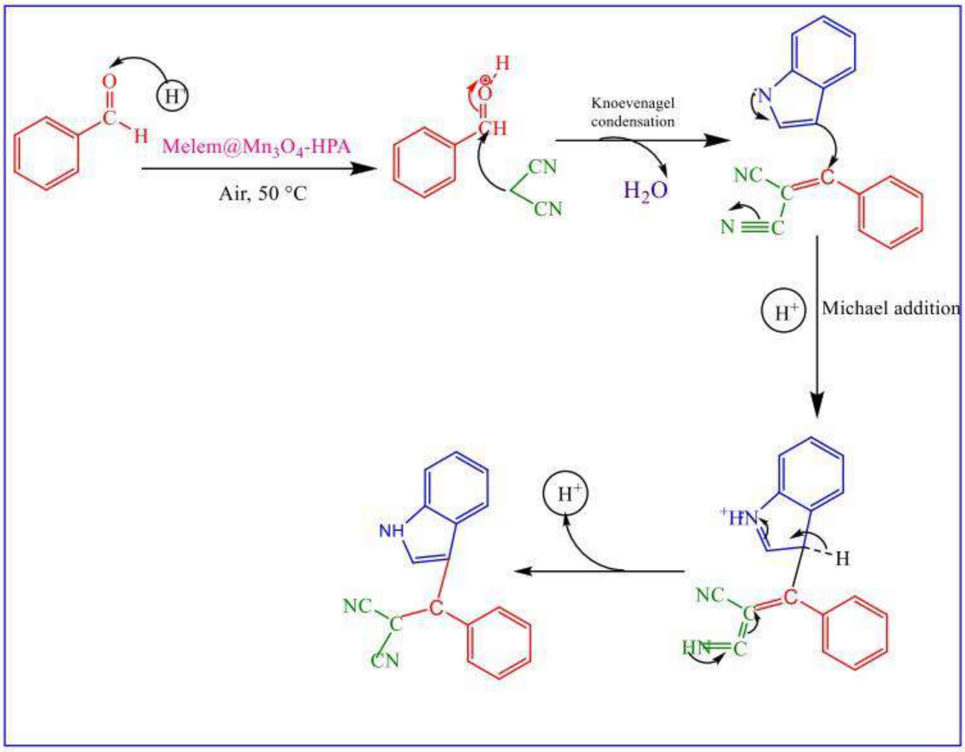

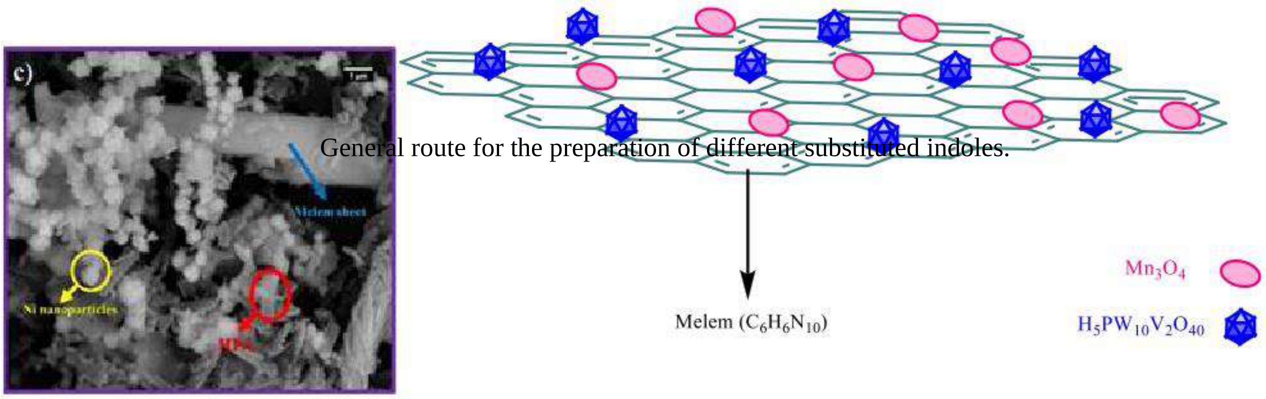

General route for the preparation of different substituted indoles.

Fabrication of a new magnetic nanocatalyst designed by Flaxseed mucilage and reduced graphene oxide aerogel for synthesis of polyhydroquinolines

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Over the last few years, the strategy of using plant extracts for green synthesis approaches has been gaining attention due to the elimination of toxic chemicals used and applying eco-friendly routes. Among a diversity of plant species, rich and valuable sources of polysaccharide hydrocolloids known as plant-based mucilages have been long-lasting of interest. These jelly-like structures with biodegradability, biocompatibility, and non-toxicity are extracted by soaking the seed hull or other herbal parts of plants treated with water. Given the chemical standpoints, the formulation of mucilages consists of large molecules such as carbohydrates and particular bioactive compounds [1]. Mucilages as functional ingredients are incorporated into the catalyst industry and food formulation due to their thickening property, emulsification mechanism, viscosity, and ease of modification. On the other hand, compared to other plant-based biopolymers, to design and formulate new hydrogel networks, it has been confirmed that mucilages as primary biopolymers or cross-linking agents have indicated better performance with higher stability [2]. Graphene-based aerogels, the known lightest three-dimensional structures, have been a longstanding of interest due to their unique and exceptional features such as remarkable adsorption capacity, specific surface area, electrical conductivity, thermal resistance, and high mechanical strength [3]. Particularly, this multifunctional structure can act as highly potent catalytic support to design and fabricate advanced and newly discovered compositions [4]. In this current study, a new magnetic nanocomposite was designed and synthesized based on the extraction of Flaxseed mucilage, transformation of graphene oxide (GO) sheets to reduced graphene oxide (rGO) aerogel, and in-situ magnetizing the composition of these two structures. Following the chemical and structural characterization of magnetic Flaxseed mucilage/rGO aerogel nanocomposite (FT-IR, EDX, FE-SEM, XRD, TG analyses), by considering the paramount pharmaceutical aspects of polyhydroquinoline derivatives, its catalytic activity was evaluated in one-pot asymmetrical Hantzsch condensation reaction. A partial amount of this magnetic nanocatalyst with a high synergetic catalytic effect leads to form a high percentage of yields of products at room temperature and a shorter reaction time.

Keywords: Mucilage; Reduced graphene oxide aerogel; Flaxseed; Magnetic nanocomposite; Polyhydroquinoline

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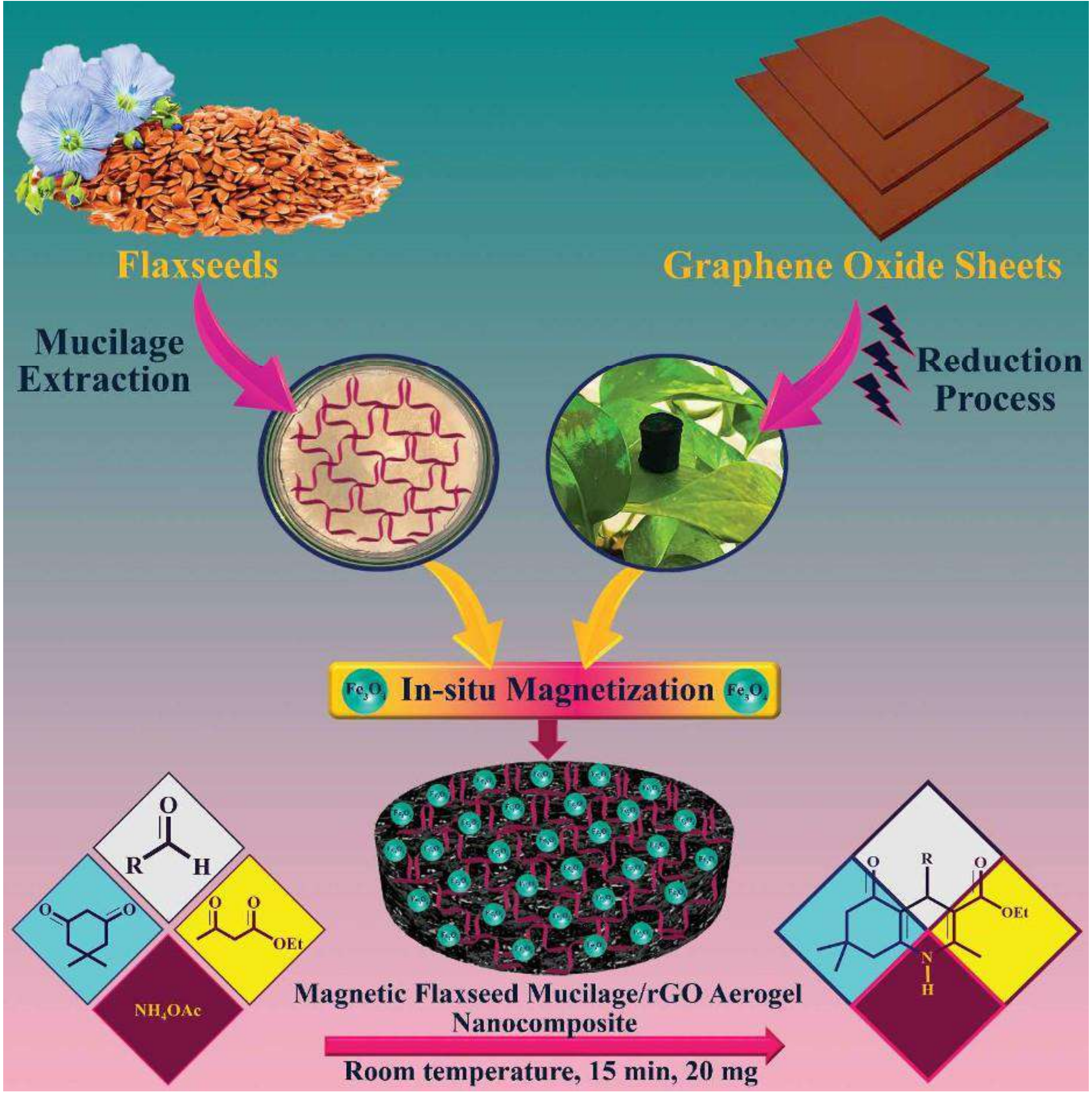

Scheme 1 Synthesis process of magnetic flaxseed mucilage/rGO aerogel nanocomposite and its catalytic activity in synthesis of polyhydroquinoline derivatives

Preparation, characterization, and catalytic application of Ionic liquid/SO_3H in the synthesis of 1,4-dihydropyridine derivatives

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Keyword: Ionic Liquid, 1,4-dihydropyridine, Hantzsch reaction, Ionic Liquid/SO_3H.

This study presents the preparation and characterization of Ionic liquid/SO_3H and its application in the synthesis of 1,4-dihydropyridine derivatives as a catalyst. Ionic liquid/SO_3H was synthesized through a facile method, and it was characterized using techniques such Fourier-transform infrared spectroscopy. The catalytic performance of the Ionic liquid/SO_3H was evaluated in the Hantzsch reaction, a widely utilized multicomponent reaction in organic synthesis. Remarkably, it exhibited excellent catalytic activity, high selectivity, and superior recyclability in promoting the Hantzsch reaction, showcasing its potential as a promising catalyst for sustainable and efficient synthesis processes.

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