بسم الله الرحمن الرحیم

Dear Participant

Welcome to 23rd Iranian Inorganic Chemistry Conference, that will be held during November 6 and 7, 2024 (Aban 16 and 17, 1403) at the Department of Chemistry, Faculty of Science, University of Qom with the collaboration of the Iranian Chemical Society to expand upon the knowledge and technology in inorganic chemistry, dependent fields and applications in industries, nanotechnology, environment, etc. The scientific program covers a wide variety of topics in various fields of inorganic chemistry. The submitted papers of esteemed colleagues, students, researchers, and industrialists will be reviewed by the scientific committee and presented in two formats of speech and poster. The scientific and organizing committee would like to express their deep gratitude to all authors for their contribution in this conference. We hope that you will have a wonderful experience in Qom city and University of Qom will stay in your memories forever. We would like to heartly appreciate the Chancellor, Finance Vice Chancellor and Research Vice Chancellor of the University of Qom, and Iranian Chemical Society, Scientific Committee, Department of Chemistry and Organizing Committee for their valuable contribution.

With the best regards

Akbar Rostami-Vartooni

Associate Professor in Inorganic Chemistry

The Scientific Secretary of 23rd Iranian Organic Chemistry Conference

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برنامه زمان بندی بیست و سومین کنفرانس شیمی معدنی در روز چهارشنبه ۱۶ آبان ۱۴۰۳ (سالن شیخ مفید)

ردیف	شرح			زمان
۱	صبحانه، رستوران دانشگاه قم			۷:۰۰ – ۸:۰۰
۲	**مراسم افتتاحیه**	تلاوت آیات قرآن کریم - سرود جمهوری اسلامی ایران اجرای کلیپ معرفی دانشگاه قم		۸:۰۰ – ۸:۲۰
		خیر مقدم رییس یا معاون پژوهشی دانشگاه		۸:۲۰ – ۸:۳۰
		گزارش دبیر علمی کنفرانس		۸:۳۰ – ۸:۴۵
		سخنرانی دبیر انجمن شیمی تجلیل از شیمیدان معدنی برجسته کشور		۸:۴۵ – ۹:۱۰
		سخنرانی شیمیدان معدنی برجسته		۹:۱۰ – ۹:۴۵
۳		**پذیرایی و بازدید از پوسترها**		۹:۴۵ – ۱۰:۴۵
	هیات رئیسه	**سخنران**	**عنوان سخنرانی**	
۴	دکتر مجید پورمقدم دکتر مجید مقدم	شرکت پتروشیمی نوری	دستاوردهای پتروشیمی در حوزه کاتالیست، انرژی و هوش مصنوعی	۱۰:۴۵ – ۱۱:۰۵
		شرکت فولاد غرب آسیا	کاربرد علم شیمی در صنعت فولاد	۱۱:۰۵ – ۱۱:۲۵
		شرکت توسعه منابع انرژی	معرفی حوزه‌های کاری سازمان توسعه منابع انرژی	۱۱:۲۵ – ۱۱:۴۵
۵		**نماز و ناهار**		۱۱:۴۵ – ۱۳:۳۰
۶	دکتر محمدمهدی نجف‌پور دکتر غلام‌حسین محمدنژاد	شرکت مصباح انرژی	استفاده از کاتالیست‌ها در فرایندهای تبادل ایزوتوپی	۱۳:۳۰–۱۳:۵۰
		شرکت معدن منگنز ونارچ	فعالیت های معدن منگنز در سال های گذشته و آینده نگری در حوزه شیمی	۱۳:۵۰–۱۴:۱۰
		شرکت شیمی اکسیر بوستان	جایگاه کودهای معدنی در کشاورزی	۱۴:۱۰–۱۴:۳۰
		دکتر مجید پورمقدم (پژوهشگر برتر وزارت صمت)	ایران قدرت معدنی پنهان جهان، تحلیلی بر ۷۵ نوع ماده معدنی ایران	۱۴:۳۰–۱۴:۵۰
		دکتر شهریار غمامی (هیأت علمی دانشگاه بین المللی قزوین)	Preparation of New Nano Inorganic Materials and Study of Their Biological Properties: (Anti-Cancerand Antibacterial) & There's Plenty of Room at the Bottom	۱۴:۵۰–۱۵:۱۰
۷		**پذیرایی و بازدید از پوسترها**		۱۵:۱۰–۱۶:۰۰
۸	دکتر شهریار غمامی دکتر حمیدرضا شهسواری	دکتر صابر عمو رسولی (موسس و رییس سابق خانه معدن استان قم)	فرصت های اشتغال و سرمایه گذاری پیرامون مواد معدنی و موقعیت گردشگری دریاچه نمک قم	۱۶:۰۰–۱۶:۲۰
		شرکت پالایش نفت امام خمینی (ره) شازند	کاربرد کاتالیست ها در صنعت پالایش نفت	۱۶:۲۰–۱۶:۴۰
		شرکت فاتحان علم و فناوری فخرا	معرفی مسیر راه اندازی کسب و کار دانش بنیان در حوزه شیمی	۱۶:۴۰–۱۷:۰۰
		زیست بوم علم و فناوری کساء	توسعه زنجیره ارزش باطله‌های معدنی	۱۷:۰۰–۱۷:۲۰
۹	**زیارت حرم مطهر حضرت معصومه (س) و مسجد مقدس جمکران**			۱۹:۰۰–۲۲:۰۰

برنامه زمان بندی بیست و سومین کنفرانس شیمی معدنی در روز پنج شنبه ۱۷ آبان ۱۴۰۳ (سالن شیخ مفید)

ردیف	شرح			زمان
۱	صبحانه، رستوران دانشگاه قم			۷:۰۰ – ۸:۰۰
۲	**هیأت رئیسه**	**سخنران**	**عنوان سخنرانی**	
۳	دکتر صادق صالح زاده دکتر ولی الله میرخانی	عالمه آذرنگ (دانشجوی دکتری دانشگاه صنعتی اصفهان)	Synthesis, characterization, and structure of pyrazine carboxylic acid-based carboxamide ligands and their complexes with copper (II), nickel (II), and cobalt (II) and the ligands application as fluorescence sensor	۸:۰۰ – ۸:۲۰
		دکتر حمیدرضا شهسواری (هیأت علمی دانشگاه تحصیلات تکمیلی علوم پایه زنجان)	An Organoplatinum(II) Complex Containing Polycyclic Aromatic Hydrocarbon Ligand: Synthesis and Characterization	۸:۲۰ – ۸:۴۰
		دکتر علی مرسلی (هیأت علمی دانشگاه تربیت مدرس)	Production of water from air using metal-organic frameworks	۸:۴۰ – ۹:۰۰
		دکتر رضا کیا (هیأت علمی دانشگاه صنعتی شریف)	The n → π^* Interactions in Metal-Carbonyl Complexes: A Case Study on Re(CO)3 Core Complexes	۹:۰۰ – ۹:۲۰
		دکتر نیلوفر اکبرزاده (هیأت علمی دانشگاه سیستان و بلوچستان)	Metal-organic framework based voltammetric sensor for simultaneously detection of drugs	۹:۲۰ – ۹:۴۰
۴	پذیرایی و بازدید از پوسترها			۹:۴۰ – ۱۰:۳۰
۵	دکتر علی مرسلی دکتر ابوالقاسم کاهانی	دکتر مریم غیاثیان آرانی (هیأت علمی دانشگاه کاشان)	Electrode material based on sol-gel synthesized Ca-Mn-O nanostructures for electrochemical hydrogen storage application	۱۰:۳۰ – ۱۰:۵۰
		دکتر صادق صالح زاده (هیأت علمی دانشگاه همدان)	Cooperativity of metal-ligand bonds and trans-influence of ligands	۱۰:۵۰ – ۱۱:۱۰
		دکتر رضا کشاورزی (هیأت علمی دانشگاه اصفهان)	Perovskite materials in solar cells and water splitting	۱۱:۱۰ – ۱۱:۳۰
		فاطمه سلیمانی راوندی (دانشجوی دکتری دانشگاه دامغان)	A novel complex of Co(II) with pyrazine-2-carboxamide derivative ligand; synthesis, characterization & single crystal X-ray diffraction studies	۱۱:۳۰ – ۱۱:۵۰
۶	نماز و ناهار			۱۱:۵۰ – ۱۳:۳۰
۷	دکتر مرتضی منتظرظهوری دکتر نیلوفر اکبرزاده	دکتر رضوان رحیمی (دانشجوی پسا دکتری دانشگاه اراک)	Periodic DFT insights into a promising nanosheet for hydrogen storage applications	۱۳:۳۰ – ۱۳:۵۰
		دکتر ابوالقاسم کاهانی (هیأت علمی دانشگاه کاشان)	Unexpected preparation of polythiocyanogen $(SCN)_n$ in the solid state at room temperature	۱۳:۵۰ – ۱۴:۱۰
		گفتمان (بحث آزاد)	ارایه راهکارهای ارتباط موثرتر با صنعت، بررسی نقش مقالات در جایگاه علمی کشور، تغییر برخی سرفصل های دروس شیمی معدنی در جهت کیفیت بهتر آموزش و ...	۱۴:۱۰ – ۱۴:۴۰
۸	**پذیرایی و بازدید از پوسترها**			۱۴:۴۰ – ۱۵:۳۰
۹	مراسم اختتامیه			۱۵:۳۰ – ۱۶:۴۵

** سه دقیقه از زمان هر سخنرانی به پرسش و پاسخ اختصاص دارد.**

Synthesis of Efficient Porous Nanocomposite Based on Metal-Organic Framework UiO-66-NH_2 Coated with APTMS/5-Aminotetrazole/Au-NPs for Preparation of Propargyl Amines

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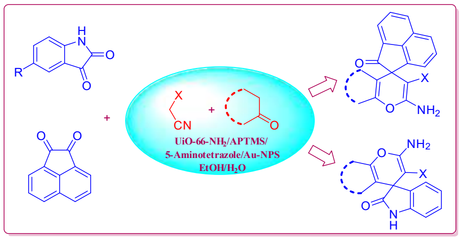
Keywords: Nano-structures, Porous Metal Organic Frameworks, Propargyl Amine, Gold-nano Particles

In this paper, a highly efficient and reusable catalyst through step-by-step post-synthesis modification of UiO-66-NH_2 metal-organic framework (MOF) was supported with nitrogen-rich as organic ligand in order to synthesis of catalyst named UiO-66-NH_2 @ 5-aminotetrazole/Au-NPs [1]. This research is motivated to identify newly synthesized MOF nano-catalyst through metal-organic framework UiO-66-NH_2 with amino group (-NH_2) as an efficient MOF functionalized with 5-aminotetrazole and stabilization *via* Gold – nanoparticles also an efficient catalyst UiO-66-NH_2 @ 5-aminotetrazole @ Au-NPs as a heterogeneous catalyst has been applied to perform of preparation propargyl amines which have been investigated (Scheme 1). The proposed catalyst represented superior catalytic performance for promoting the preparation propargyl amines 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 Gold-nanoparticles. In addition, the suggested catalyst represented excellent reusability with no remarkable loss in activity up 9 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-NH_2/APTMS/5-Aminotetrazole/Au – nanocomposite.



Scheme 1: An efficient one-pot synthesis of functionalized spirochromenes.

References

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Computational design of a potential anode material for Mg ion battery through DFT calculations

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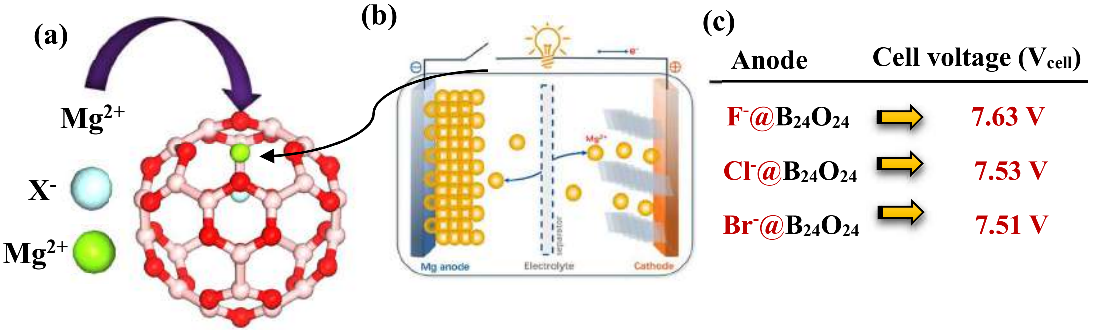
Keywords: Mg-ion batteries; $B_{24}O_{24}$ nanocage; Anode

Rechargeable magnesium batteries are considered a promising option for reversible energy storage when compared to lithium battery systems[1]. This is due to the abundant availability of magnesium resources, improved chemical stability of metallic magnesium in humid and oxygen-containing environments, and higher volumetric capacity. The present theoretical study investigated the adsorption of Mg and Mg^{2+} moieties on the $B_{24}O_{24}$ nanocage. The obtained structures were optimized using Grimme's dispersion corrections at the GGA/PBE/DNP computational level[2]. The cell voltage (V_{cell}) was then calculated for all the desired systems using the Nernst equation. This equation demonstrates that the strong adsorption between the Mg^{2+} cation and the nanocage, along with the weak adsorption of Mg metal with the $B_{24}O_{24}$ nanocage, results in a more negative ΔG_{cell} and a high V_{cell} of 4.45 V. Since maximizing V_{cell} has been the objective of this research, the performance of halides encapsulated in the $B_{24}O_{24}$ nanocage was investigated as the anode material for MIBs (Figure 1(a, and b)). The V_{cell} values for X^-@cage exhibit a significant increase compared to the pristine $B_{24}O_{24}$ nanocage, surpassing the performance of some previously reported anode materials (Figure 1(c)). The findings from this research could aid in the design of new boron-oxygen-based materials with higher cell voltage for MIBs technology.



Anode		Cell voltage (V_{cell})
F^-@$B_{24}O_{24}$	⇨	7.63 V
Cl^-@$B_{24}O_{24}$	⇨	7.53 V
Br^-@$B_{24}O_{24}$	⇨	7.51 V

Figure 1. (a) Encapsulated $B_{24}O_{24}$ cage with halides (X^- = F^-, Cl^-, and Br^-), (b) schematic of Mg-ion battery, and (c) V_{cell} values of the X^-@cage.

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Sensing and delivery of an anticancer drug over porous hexagonal boron oxide monolayer using DFT approach

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Keywords: B_3O_3; Carmustine; Anticancer drug; Drug delivery; Drug release

The present study explores the targeted drug-carrying and detecting properties of the carmustine anticancer drug using a pristine B_3O_3 sheet. This planar nanosheet is known to be suitable for biomedical applications and has been synthesized experimentally [1]. In this work, all DFT-D calculations were performed using Grimme's van der Waals (vdW) correction by utilizing DMol^3 software. The calculations were carried out at the GGA/PBE level using a localized double-numerical basis with polarization functions (DNP). Hirshfeld charge analysis [2] confirms the transfer of charge from the carmustine anticancer drug to the sheet. In the most stable configuration, the drug-loaded on the B_3O_3 sheet exhibits adsorption energy values of -1.09 eV in the gas phase and -0.58 eV in the water phase. The parallel position represents the most stable interaction between the drug and the surface. In the absence of radiation, the calculated recovery times at 306 K (normal cell temperature) and 310 K (brain tumor tissue temperature) are 3.7×10^{-3} and 2.8×10^{-3} seconds, respectively. The DMol^3 module was used to investigate the release of the drug by the final complex near brain tumor cells. The molecular dynamics (MD) analysis was conducted using the NVT ensemble at 310 K, with a time step of 1 fs in 2000 steps. Additionally, a giant thermostat of generalized Gaussian moments (GGM) was employed. According to the MD results, the carmustine anticancer drug is released from the nanocarrier when it is adsorbed on the pristine B_3O_3 substrate. This release occurs near tumor cells, which allows for targeted therapeutic intervention (Figure 1).

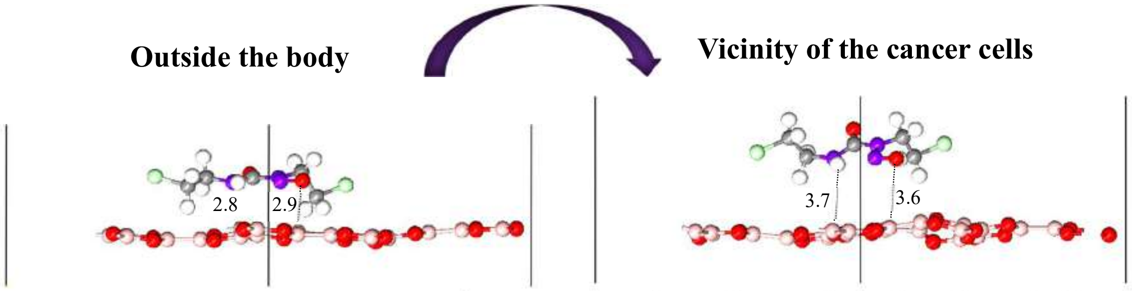

Figure 1: Optimized geometry in Å, for the carmustine anticancer drug adsorption on B_3O_3 surface in the outside the body and 310 K (Tumor tissue temperature) for the S1 complex as a most stable complex.

References

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Periodic DFT insights into a promising nanosheet for hydrogen storage applications

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Keywords: B_4CN_3 nanosheet; Hydrogen storage; DFT periodic study.

The present research focuses on the potential of a two-dimensional B_4CN_3 nanosheet for hydrogen storage. Previously, the stability of the B_4CN_3 nanosheet has been confirmed through molecular dynamics and phonon spectra calculations [1]. In the present study, we have confirmed that this nanosheet has a high capacity for storing hydrogen. The B_4CN_3 monolayer meets the necessary conditions to be used as a hydrogen storage material. DFT-D calculations were performed using Grimme's scheme with DNP plane-wave basis sets. These calculations were carried out at the GGA/PBE computational level using the DMol^3 software in the Materials Studio package [2]. The B_4CN_3 ($6H_2$) medium can store up to 11.0 wt%, surpassing the hydrogen storage goals set by the USDOE (5.5 wt% by 2020). The admissible range of adsorption energy for H_2, which is practically efficient, is between 0.1 and 0.6 eV [3]. Additionally, the average adsorption energy of 0.227 eV/H_2 falls within the ideal range, ensuring faster adsorption and desorption process (Figure 1). The B_4CN_3 ($6H_2$) framework's desorption temperature is 291 K (Figure 1). One significant advantage of this material is that it does not require doping for hydrogen storage under ambient conditions, eliminating the need for a complex and expensive doping process.

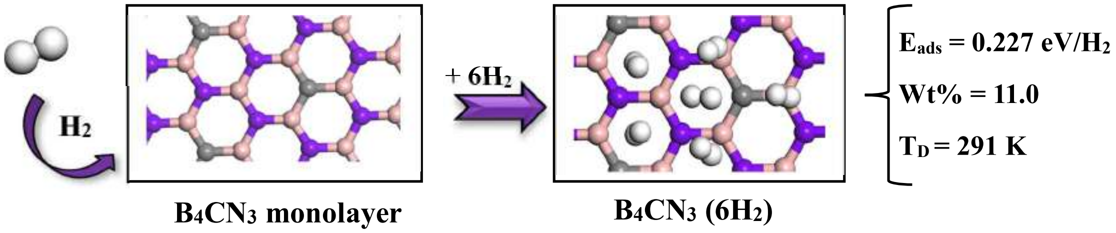

Figure 1. Hydrogen storage over the B_4CN_3 nanosheet up to $6H_2$ molecules with an adsorption energy of 0.227 eV and massive hydrogen storage capacity of 11.0 wt% with a desorption temperature of 291 K.

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Perovskite materials in solar cells and water splitting

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Keywords: Perovskite materials, Solar cells, Water splitting

Perovskite Solar Cells: Perovskite solar cells (PSCs) have shown remarkable progress due to their high efficiency and low production costs. This type of cell has a perovskite photo-absorbing layer sandwiched between electron and hole transport layers. The structure allows for efficient light absorption and charge separation, leading to high power conversion efficiencies. Recent advancements have focused on improving the stability and scalability of PSCs, addressing issues such as moisture sensitivity and long-term performance degradation [1][2].

Water Splitting: A PEC cell uses perovskite materials to split water into hydrogen and oxygen to convert solar energy into chemical energy. A minimum thermodynamic voltage of 1.23 V is required for this process, but practical devices often require higher voltages due to kinetic barriers. A perovskite is an ideal candidate for this application due to its tuneable bandgaps and high absorption coefficients. Integrated halide perovskite PEC cells have achieved solar-to-hydrogen efficiencies exceeding 20%, demonstrating their potential for efficient green hydrogen production [1][3][4].

Multi- Applications: Water-splitting technologies can be combined with perovskite solar cells to produce direct fuel from solar energy. By using hybrid systems, energy conversion efficiency can be improved and sustainable energy solutions can be offered. Future research is directed towards enhancing the stability of perovskite materials, developing cost-effective catalysts, and optimizing device architectures for better performance and durability [1][2][5].

In summary, perovskite materials hold great promise for advancing solar energy and water-splitting technologies, contributing to the development of efficient and sustainable energy systems.

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Synthesis, characterization, and application of nanoporous metal-organic frameworks (MOFs) combined with quantum dots nanoparticles and carboxylated graphene oxide

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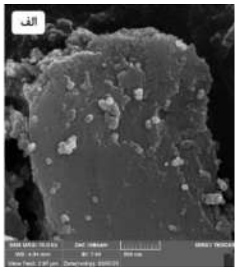
Keywords: Metal-Organic Framework, Quantum dots, Graphene oxide, CdS/HKUST-1 composite

The combination of QDs and MOFs leads to good dispersion, high stability, and photocatalytic activity. In the CdS/HKUST-1 composite, CdS QDs were decorated on the MOFs, so that, compared with the pure MOF materials, the porosity and specific surface area of the CdS/HKUST-1 composite are reduced (**scheme 1**)[1]. The UV-Vis analysis result shows that methylene blue's absorption and degradation by the CdS/HKUST-1 composite was about 87%. From this, the analyte is absorbed in the aqueous sample. In this study, HKUST-1[2] was synthesized using the hydrothermal method. In addition, CdS, and CdS/HKUST-1[3] composite were prepared by ultrasonic method. Also, Graphene oxide (GO), the oxidation product of graphene, has a large specific surface area, was prepared by Hummer's method [4].In this research, carboxylated graphene oxide is supposed to be added to this composite, and the result of its photocatalyst activity should be investigated.



Scheme 1: FE-SEM image of CdS/ HKUST-1 composite

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Adsorption of an azo dye over B_3O_3 monolayer: A DFT study

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Keywords: B_3O_3 monolayer, Solar cell, DSSC, DFT study

Dye-sensitized solar cells (DSSCs) are third-generation solar cells. They are made with inexpensive materials and have a simple manufacturing process. Grátzel and O'Regan discovered DSSCs in 1991 [1]. In DSSCs, light energy is converted into electrical energy through dye adsorption on the semiconductor's surface. The objectives of this DFT study are to investigate the adsorption properties of the p-methyl red molecule on the pristine B_3O_3 semiconducting sheet. Previously, the B_3O_3 sheet has been synthesized experimentally [2]. This research aims to assess the potential application of this combination in DSSC. All calculations were conducted by using $DMol^3$ code [3]. The electron exchange and correlation were treated using the GGA/PBE functional with Grimme's van der Waals correction. The adsorption energy of the dye on B_3O_3 ranges from -0.25 to -1.48 eV. The dye adsorption on the semiconductor enhances the electrical conductivity, photocatalytic property, and voltage during battery operation. This enhancement becomes more pronounced as the energy gap narrows. Additionally, the adsorption causes a 50 to 57% change in the percentage of band gap energy in the sheet. The dye molecule is found to adsorb in two forms on the B_3O_3 sheet (Figure 1 (a and b)), with the complexes of the trans-isomer displaying more negative E_{ads} of -1.48 eV (Figure 1 (c)), making them more stable compared to the cis-isomer complexes (-1.41 eV). Overall, the results of this study suggest that the investigated substrate holds promise for potential application in DSSC when paired with a desired dye molecule.

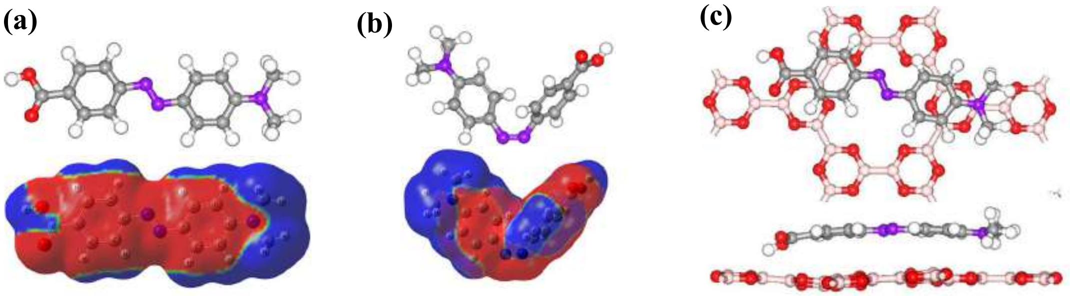

Figure 1: P-methyl red dye molecules in (a) trans and (b) cis isomers and MEP surface. (c) Top and side views of the stable complex of dye molecule of trans-P-methyl red adsorbed on the B_3O_3 nanosheet.

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Efficient and sensitive adsorption of typical free radicals over covalent triazine framework through DFT calculations

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Keywords: CTF, NO, NO_2, HO_2, Periodic DFT study

The adsorption and detection performance of pristine covalent triazine framework (CTF) for three free radicals (NO_2, NO, and HO_2) were investigated using DFT calculations. Previously, CTFs were synthesized from the dimerization of simple and inexpensive aromatic nitriles in molten $ZnCl_2$. In recent years, numerous applications of CTFs have been reported [1]. The release of nitrogen oxides is a result of combustion at high temperatures, such as from vehicle exhaust and boiler exhaust. Among these nitrogen oxides, NO_2 radical is particularly dangerous, as it also contributes to the formation of ozone in the troposphere [2]. These pollutants have various negative impacts, including the occurrence of acid rain, reduced visibility in the atmosphere, acidification, and eutrophication of surface water. Additionally, the presence HO_2 contributes to the depletion of ozone [3]. All DFT calculations are conducted using the DMol^3 code at the GGA/PBE/DNP computational level. The moieties were found to adsorb on the CTF (Figure 1(a)) with adsorption energies ranging from -0.05 to -0.46 eV. The higher E_{ads} of the HO_2 radical compared to the other two radicals is attributed to hydrogen bond interactions between the H atoms of the HO_2 radical and the N atom of the CTF. The conductivity change values for the NO_2/CTF, NO/CTF, and HO_2/CTF complexes are calculated to be 2×10^{11}, 4×10^{19}, and 1×10^{12}, respectively. The significant change in conductivity (%ΔE_g) upon adsorption of the studied radicals indicates the potential of the CTF for detecting radicals (Figure 1(b)). Based on the results, the pristine CTF sheet can serve as a predominant adsorbent and a potential sensor for these radicals in certified operations.

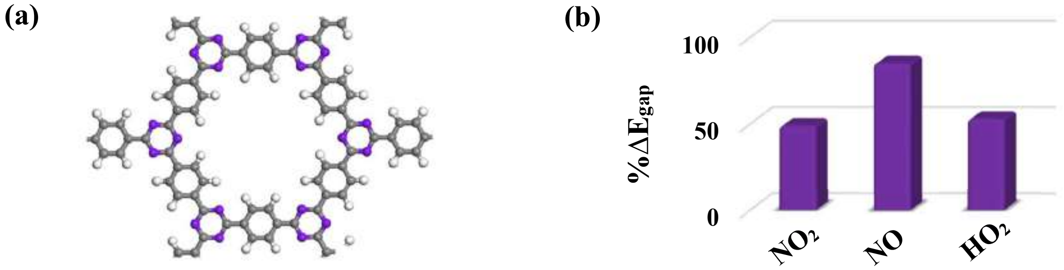

Figure 1. (a) Optimized structure of the pristine CTF, (b) the percentage change in the E_g (%ΔE_g) of the NO_2/CTF, NO/CTF and HO_2/CTF complexes.

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DFT study of a promising anode material for lithium-ion batteries

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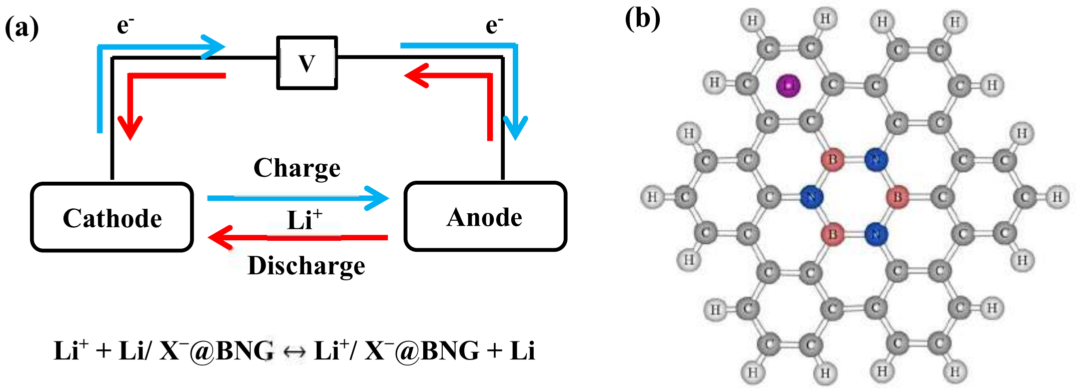
Keywords: Li-ion batteries; Borazine doped nanographene; Anode

Li-ion batteries (LIBs) are widely regarded as the most superior energy storage systems available. Figure 1 (a) schematically illustrates the process of charging and discharging in LIBs. This is attributed to their unique properties, such as their compactness, lightweight nature, long cycle life, environmental compatibility, design flexibility, and their ability to operate at high voltages [1]. The potential application of borazine-doped nanographene (BNG) as an anode in LIBs has been investigated using DFT study. Krieg et al. have synthesized BNG [2]. All calculations in this study is performed at the GGA-PBE/DNP computational level via DMol^3 code. The interaction between Li and Li^+ cations occurs over the outer rings of the BNG nanostructure (Figure 1(b)), with adsorption energy values of -25.2 and -47.9 kcal/mol, respectively. This interaction results in an electrochemical cell voltage (V_{cell}) of 0.99 V. Furthermore, the performance of LIBs is significantly improved by decorating BNG with halides. This strategy increases V_{cell} from 0.99 V to 3.98, 1.54, and 1.62 V for BNG/F^-, BNG/Cl^-, and BNG/Br^- complexes, respectively. The calculated V_{cell} of 3.98 V for $BNG\cdots F^-$ is greater than the values reported in previous literature for different nanostructures used as anode materials in LIBs. In conclusion, we hope that the results of this research will be utilized in the design and manufacturing of more efficient lithium batteries.



$Li^+ + Li/\ X^-@BNG \leftrightarrow Li^+/\ X^-@BNG + Li$

Figure 1. (a) Schematic of the charging and discharging process and the overall reaction for Li-ion batteries, (b) Li···BNG complex.

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Computational features of B_3O_3 monolayer as a potential nanocarrier for drug delivery of an anticancer drug

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Keywords: B_3O_3; TEPA; Anticancer drug; Drug delivery; Drug release.

This research investigates the uptake and release of the N, N′, N″-triethylenephosphoramide (TEPA) anticancer drug by pristine B_3O_3 nanosheets through periodic DFT computations. TEPA drug exhibits active anti-proliferative properties against different types of tumors[1]. The B_3O_3 hexagons have a planar structure with strong covalent B–B bonds and exhibit six-fold symmetry, as confirmed by experimental[2] evidence. The DFT-D calculations were performed using Grimme's van der Waals (vdW) correction with the DNP at the GGA/PBE level, employing the DMol[3] code[3]. The most stable configuration of drug adsorption occurs when the C atom of the drug's triangular ring interacts with the B atom of the B_3O_3 nanosheet. The drug and nanosheet interaction is strong in both the gas phase (-1.468 eV) and the aquatic medium (-1.395 eV). Interestingly, the adsorbed drug on B_3O_3 exhibits significant weakness in acidic environments typically found in cancer tissues (Figure 1). This suggests that the pristine B_3O_3 could serve as an excellent substrate for drug carriers in the targeted treatment of malignant growth cells.

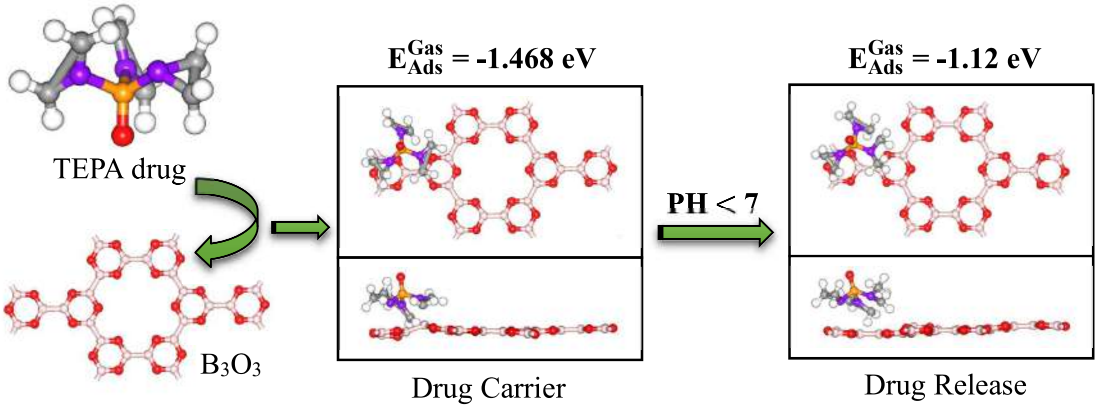

Figure 1. Adsorption, carrier, and release of the TEPA drug on the B_3O_3 sheet by mentioning the adsorption energy during adsorption and in the acidic environment near cancer tissues.

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Efficient Synthesis of Polyhydroquinolines Catalyzed by 4-Sulfophthalic Acid Grafted on Silica-Coated Magnetic Zirconium Ferrite Nanoparticles

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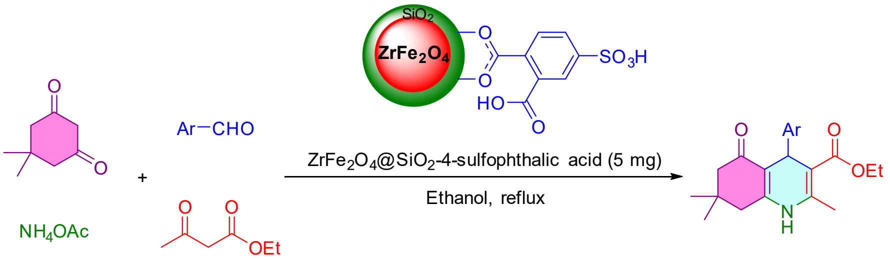
Keywords: Solid acid cataklyst, 4-Sulfophthalic Acid; $ZrFe_2O_4$, Polyhydroquinolines

Solid acid catalysis has emerged as a sustainable and efficient approach for multicomponent reactions (MCRs) [1-3]. In this study, we developed a novel heterogeneous catalyst by immobilizing 4-sulfophthalic acid, a green organic acid, onto silica-modified zirconium ferrite nanoparticles. This catalyst exhibited exceptional performance in the synthesis of polyhydroquinoline derivatives via MCRs, affording excellent yields in remarkably short reaction times in ethanol. A comprehensive investigation of the catalyst's properties, including acidity, pore structure, and surface area, revealed their crucial roles in optimizing catalytic activity. The combination of high efficiency, eco-friendliness, and recyclability makes this catalytic system a promising candidate for sustainable chemical processes.



Scheme 1: Suzuki reaction over the catalysis of $ZrFe_2O_4@SiO_2$-4-sulfophthalic acid (5 mg).

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Synthesis of $ZrFe_2O_4$@UiO-66-NH_2 Pd(0) as an nanomagnetic MOF catalyst for Suzuki reaction

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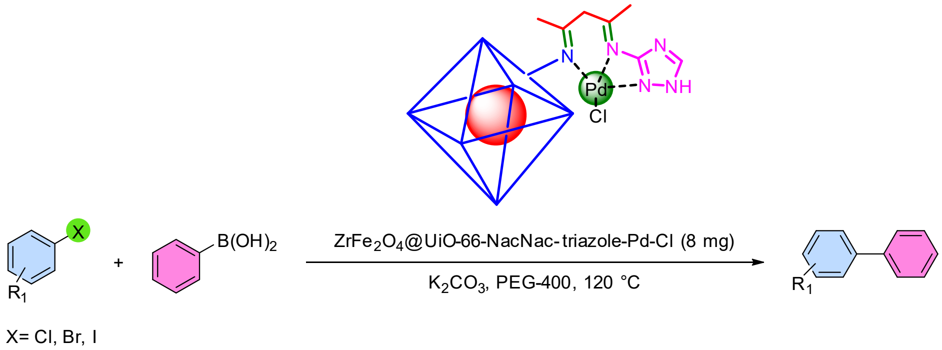
Keywords: Nano magnetic MOF, $ZrFe_2O_4$@UiO-66-NH_2, Palladium complex, Suzuki reaction

Heterogeneous catalysis is a cornerstone of chemical industry, underpinning over 80% of chemical product synthesis. Its significance necessitates a comprehensive understanding of fundamental principles and practical applications among chemists and chemical engineers. Cross-coupling reactions, pivotal in constructing C-C bonds for drug development, present a critical challenge in achieving both efficiency and environmental sustainability [1,2]. In response, we developed a novel magnetic MOF-based catalyst. This catalyst integrates a magnetic $ZrFe_2O_4$ core with UiO-66-NH_2, providing a robust platform for immobilizing a palladium complex as the active catalytic site (Scheme 1). Our results demonstrate exceptional catalytic performance in the coupling of aryl halides and arylboronic acids. The catalyst exhibited remarkable stability, maintaining high activity over eight consecutive cycles without appreciable loss of efficiency. This robust and recyclable catalyst offers a promising avenue for sustainable and scalable cross-coupling reactions, potentially contributing to greener and more efficient drug synthesis processes.



Scheme 1: Suzuki reaction over the catalysis of [$ZrFe_2O_4$@UiO-66-NacNac-triazole-Pd-Cl].

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Photocatalytic activity and self-cleaning properties of transparent ZnO/GO composite coatings

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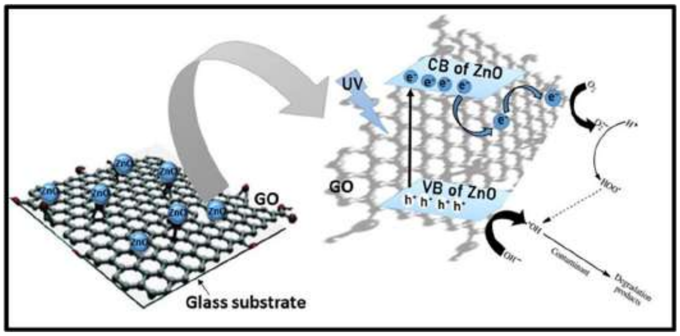
Keywords: GO, ZnO, Transparent coating, Superhydrophilic surface, Self-cleaning.

In this study, we synthesized transparent composite thin films composed of zinc oxide (ZnO) and graphene oxide (GO) using the sol-gel method. These ZnO/GO thin films were deposited onto glass substrates via the dip-coating technique. The resulting transparent ZnO/GO composite exhibited remarkable photoactivity and wettability, making it highly effective for self-cleaning applications [1]. The reduction in the band gap energy of the ZnO/GO composite, compared to pure ZnO, can be attributed to the presence of GO sheets. Specifically, photoexcited electrons from the conduction band of ZnO migrate to the surface of GO across the ZnO/GO interface (**Scheme 1**). Additionally, the presence of GO inhibits the aggregation of ZnO nanoparticles, leading to an increased photodegradation rate of pollutants. Furthermore, the GO sheets significantly influence the surface wettability, resulting in superhydrophilicity properties [2]. Notably, even after photodegradation tests, the film maintains proper adhesion integrity, and its superhydrophilicity persists even after scratch tests. Importantly, all coatings remain sufficiently transparent, avoiding any alteration of the substrate colour.



Scheme1: The proposed reaction mechanism for the photocatalytic degradation of the pollutants in the presence of ZnO/GO composite coating.

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Amberlyst-15 catalyzed the synthesis of α-halocarboxylic acid through Esterification of chloroacetic acid

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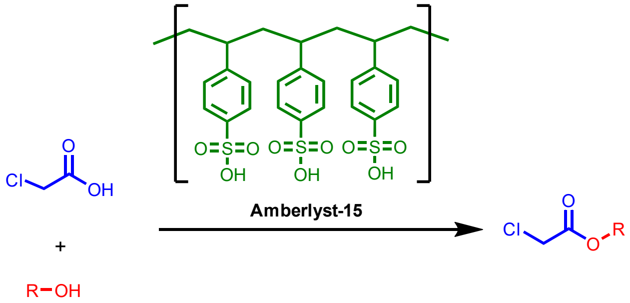
Keywords: Chloroacetic acid, Esterification, Amberlist-15 catalyst, Response Surface Methodology.

Fischer esterification regarded as the most common and widely practiced process of ester synthesis, faces serious limitations of low conversion and high reaction time attributed largely to establishment of equilibrium. Ester hydrolysis, reverse reaction to esterification, starts by supply of a byproduct- water. Several approaches have been developed to avoid equilibrium establishment and to improve overall conversion and rate of reaction, a significant difference exists between the current industrial practices and optimum esterification process/conditions [1-3]. This study describes a sustainable method for producing α-halocarboxylic acid ester derivatives from various alcohols and chloroacetic acid using Amberlyst-15 as a catalyst. The reaction conditions were optimized using response surface methodology (RSM) to maximize yield and selectivity. All starting materials are commercially available, making the process practical and scalable. The green and sustainable nature of this approach makes it promising for the production of ester derivatives (**Scheme1**).



Scheme1: Esterification of chloroacetic acid over the catalysis of Amberlyst-15.

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Oxidative addition of MeI to Pt(II) complex bearing phenanthroline derivative as N^N donor ligand: kinetic and theoretical investigation

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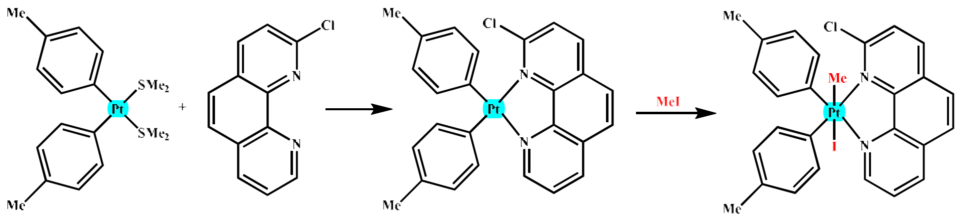
Keywords: Platinum, N^N donor ligand, Oxidative addition, Kinetic, Theoretical calculations.

One of the most important reactions in the organometallic research, the oxidative addition (OA) reaction, is also one that is essential to industry. In recent years, more research has been done on the OA in Pt(II) compounds since platinum has a large variety of stable complexes in organometallic chemistry [1]. The kinetics of Pt(II) complexes containing N^N cyclometalated ligands such as (2,2'-bipyridine) [2] and (1,10-phenanthroline *N*-oxide) [3] with different reagents such as MeI and EtI were studied. Furthermore, the mechanism of the OA reactions on these platinum complexes was studied. The new Pt(II) complex [Pt(*p*-MeC$_6$H$_4$)$_2$(phen-Cl)], **1**, phen-Cl = 2-chloro-1,10-phenanthroline, was synthesized by the reaction of [Pt(*p*-MeC$_6$H$_4$)$_2$(SMe$_2$)$_2$], **A**, and phen-Cl, **B**. MeI reagent was added to a Pt(II) complex **1** and gave a corresponding Pt(IV) complex [Pt(*p*-MeC$_6$H$_4$)$_2$MeI(phen-Cl)] **2** (**Scheme 1**). The kinetic of this reaction was studied, and the computational investigations were carried out to determine the geometry of the species involved in the suggested mechanism and energy barriers.



A B 1 2

Scheme 1. Synthetic route for the preparation of the Pt complexes.

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Harnessing Defects in Metal-Organic Frameworks for Advanced Catalysis

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Keywords: Metal-Organic Frameworks, Soft Materials, Engineering Defects, Catalyst, Lewis Acid

Metal-organic frameworks (MOFs) with engineered defects have emerged as a ground breaking class of materials, attracting significant scientific interest due to their abundant active sites and highly tunable physicochemical properties [1]. While the concept of a "perfect" MOF exists in theory, the practical synthesis of these materials invariably introduces defects, as even minor variations in reaction conditions can profoundly impact the final structure. These defects, far from being mere imperfections, can be strategically engineered to enhance MOF functionality. They manifest in various forms, including missing metal clusters, absent organic linkers, or structural rearrangements that induce dynamic behavior within the framework. The presence of defects creates open sites within the MOF structure, dramatically altering its properties and expanding its potential applications. These engineered imperfections play a pivotal role in numerous fields, including advanced catalysis, photocatalytic organic transformations, environmental pollutant remediation, detoxification of chemical warfare agents, and so on. By precisely controlling the nature and distribution of defects, researchers can tailor MOFs for specific applications, pushing the boundaries of materials science and addressing critical global challenges in energy and environmental-related applications [2]. The Knoevenagel condensation is an important organic reaction used to form carbon-carbon bonds. It typically involves the reaction between an aldehyde with an active methylene compound. In this research work, the Knoevenagel reaction was carried out in the presence of two types of MOFs as heterogeneous catalysts (**Figure 1**). Notably, the defective MOF showed superior catalytic activity compared to the pristine MOF in terms of reaction time and product yield. This study highlights the potential of defect engineering in MOFs to enhance their catalytic properties.

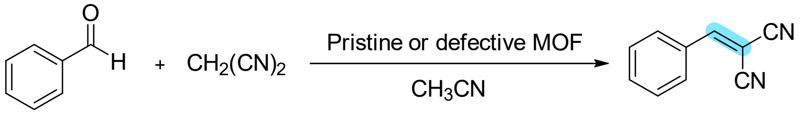

Figure 1: Knoevenagel condensation reaction catalyzed by pristine and defective MOFs.

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Interaction of Cp_2VCl_2 anticancer drug and cytosine: A DFT investigation

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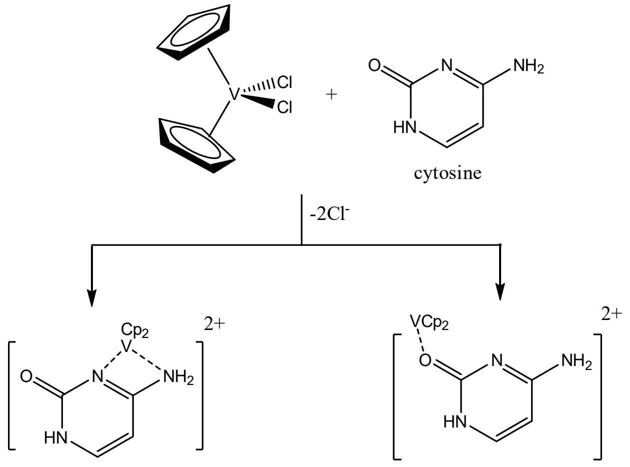
Keywords: Vanadocene dichloride, cytosine, QTAIM, EDA

Vanadocene dichloride (VDC) has been used as an anticancer drug [1-3]. In this work, the interaction of VDC and cytosine was examined at the BP86/6-311G (d,p) level of theory. Two possible modes of the binding of cytosine to VCp_2^{2+} were considered. Energetic stability of these isomers was compared. Energy decomposition analysis (EDA) and Quantum theory of atoms in molecules (QTAIM) analysis provided deep insights into the nature and the strength of the vanadocene–cytosine binding.



I

II

Scheme 1: Possible modes interactions of vanadocene dichloride and cytosine.

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UV-vis spectral evidence for strong interactions between an unfunctionalized porphyrin and TiO_2

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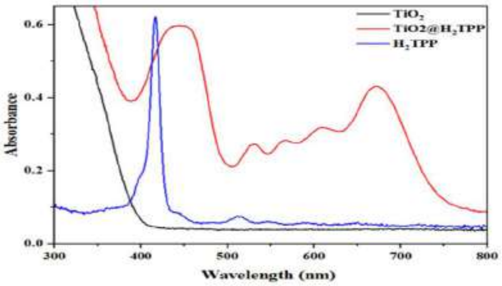
Keywords: *Meso*-tetraphenylporphyrin, Absorption bands, Anatase TiO_2, Bathochromic shift

Porphyrins are aromatic macroheterocyclic compounds with intense absorption bands in the visible region known as the Soret (400-450 nm) and Q bands (500-700 nm) [1]. The change in the wavelength of the Soret and Q bands of porphyrins has been used to provide evidence on the conformation of porphyrin core; large red shifts of the Soret and Q bands of the aromatic compounds show the distortion of porphyrin core to a nonplanar conformation [2,3]. In this study, *meso*-tetraphenylporphyrin, H_2TPP, was successfully immobilized on the surface of anatase TiO_2 in a nonpolar solvent to synthesis a green-colored porphyrin nanocomposite with bathochromic shifts in both the Soret and Q bands region. The formation of a nonplanar porphyrin moiety was evidenced by UV-vis diffuse reflectance spectroscopy (**Scheme 1**). Hydrogen bond interactions between H_2TPP and TiO_2 are probably involved in the formation of the nonplanar structure and the red shifted absorption bands of H_2TPP. It is noteworthy that the choice of solvent is crucial for the successful synthesis of $TiO_2@H_2TPP$ nanocomposites; the formation of the nanocomposites is completely prevented in polar solvents such as DMF [4].



Scheme1: Spectral changes upon the immobilization of H_2TPP on TiO_2.

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Oxidative degradation of methylene blue with nanostructured iodosylbenzene in the presence of iron porphyrins

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Keywords: Iron-porhyrins, Nano-structured Iodosylbenzene, Methylene blue, Oxidative degradation

The iron complexes of a porphyrin with cationic substituents at the *meso* positions, *meso*-tetrakis(4-methylpyridyl)porphyrin, H_2TMPy also the sulfonated derivatives of *meso*-tetrakis(4-methoxyphenyl)porphyrin, $H_2T(4\text{-}OCH_3)PP$, *meso*-tetrakis(2-chlorophenyl)porphyrin, $H_2T(2\text{-}Cl)PPS_4$ (**Scheme1**), were used as catalysts in degradation of methylene blue (MB) with bulk and nano-structured iodosylbenzene under aqueous homogeneous conditions. The nanostructured oxidant, PhIO-TEG was synthesized by controlled alkaline hydrolysis of iodobenzene diacetate in the presence of triethylene glycol monomethyl ether (TEG) as the stabilizer [1]. The decrease of size of the oxidant to nanoscale was found to increase the rate of the oxidative degradation of MB. Also, the influence of the *meso* substituents on the catalytic activity of the iron porphyrins was investigated. It is noteworthy that due to the very low solubility of most hypervalent iodine compounds, many efforts were devoted to the synthesis of more soluble and reactive I(III) and I(V) derivatives [2-4].

Scheme1: The oxidative degradation of MB in the presence of iron porphyrin and nanostructured iodosylbenzene.

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Magnetic /activated carbon obtained from raspberry bush (Rb) to remove Pb^{2+} ions from polluted water

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Keywords: Absorption, Magnetic, Activated carbon, Pb^{2+}

The lack of water around the world is one of the serious problems that the increasing population growth and the excessive use of water resources have caused to decrease the level of water on the ground. Effluents entering the environment from various human activities pose risks to living organisms [1]. Lead (Pb^{2+}) in water is harmful to humans and can cause damage to the brain and nervous system [2]. In this process, magnetic nanocomposites based on spinel ferrite and activated carbon were used. This nanocomposite has a special application in water purification technology due to its magnetic properties and simplicity in separation [3]. On the other hand, according to the results of FESEM and BET images, the diameter of pores is 2.04 nm, which had high porosity. Therefore, in this study, the raspberry plant was pyrolyzed at 600°C for two h after activation by $ZnCl_2$. After making magnetite from metal salts at a temperature of 80°C, activated carbon obtained from the raspberry plant (Rb) was added to the solution at a ratio of 1:1. After 30 min, the NaOH solution was added to the salt solution as a precipitating agent, and finally, the separation process was carried out by a neodymium magnet. Fe_3O_4/Rb nanocomposite was used to remove Pb^{2+} metal from polluted water. The results of adsorption showed that Fe_3O_4/Rb at pH=9, optimal duration of 30 min, initial concentration of 50 mg/L and at room temperature shows the greatest ability to remove Pb^{2+}. Therefore, the highest removal efficiency is 99.69% and the absorption capacity is 249.24 mg/g. Also, by comparing the results of analyzes such as XRD, Raman before and after absorption, peaks were observed at pH=9, which indicates the absorption of Pb^{2+} by Fe_3O_4/Rb nanocomposite. This adsorbent can be reused for four cycles with reduced absorption performance.

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Quantum calculations of non-covalent adsorption of gentamicin on natural single-walled carbon nanotube functionalized with COOH functional group

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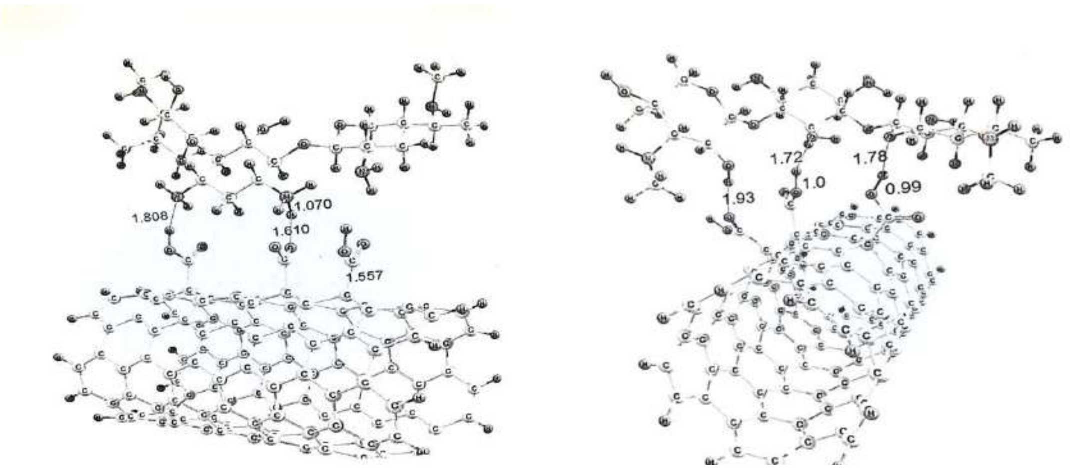
Keywords: Quantum mechanics , Swcnt , Non-covalent ,Gentamicin

Gentamicin is a commonly used antibiotic which prevents bacterial infection around the implant.It is an aminoglycoside antibiotic , and can treat many types of bacterial infections , particularly Gram-negative infection[1].

In this work , using quantum mechanics , the interaction of drug gentamicin(GEN) with natural nanotubes(NT) and COOH functionalized (NTCOOH) single carbon nanotubes (SWNTs) have been studied.All of the present calculations have been performed with the B3LYP hybrid density functional level using the GAUSSIAN03 package in gas and solution phases.[2] Quantum molecular descriptors and frontiter orbital analysis in the drug- nanotube systems were studied . It was found that binding of gentamicin with pristine (GEN/NT) in gas phase and COOH functionalized (GEN/NTCOOH) carbon nanotubes in both phases is thermodynamically favorable.(**Scheme1**) The solvation energies show that the solubility of GEN/NTCOOH is higher than GEN/NT[3].



a.(gas phase) **b.(solvent phase)**

Scheme1: Optimized structure of GEN/NTCOOH.

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Introducing one-pot synthesis of Zn-MOF based on terephthalate compounds for electrochemical applications

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Keywords: Nanomaterials, Solvothermal, Metal-Organic Framework

Metal-organic frameworks were introduced in the late 1990s by a research group under the guidance of Professor Omar Yaghi with Frey and Kitagawa at the University of California, Berkeley [1]. MOFs are a group of compounds consisting of metal ions or clusters that are coordinated with organic linkers and form one, two or three-dimensional structures. These compounds can be converted into materials with micro-nano architecture, such as carbon and its hybrids, which have porous materials with a crystalline structure and have recently attracted a lot of attention. As a class of functional porous polymers with high surface area, regular porosity, low density, tunable structures and high thermal stability, these materials are widely used in gas storage, separation, catalysis, drug delivery, electrochemical sensors, batteries, etc [2]. Due to their high surface area and permanent porosity, MOFs are used to load or encapsulate catalytically active metal nanoparticles, which can effectively prevent the re-aggregation of metal nanoparticles and facilitate catalytic efficiency (**Scheme1**). According to the explanation in the present study, we prepared Zn-MOF using $Zn(NO_3)_2 \cdot 6H_2O$, para-phthalic acid as ligand, DMF and ethanol according to reference [3].

Scheme1: Zn-MOF applications in electrochemistry.

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Defect-engineered Pore Expansion in Cu-BTC using Surfactants for Enhanced Post-synthetic Guest Loading

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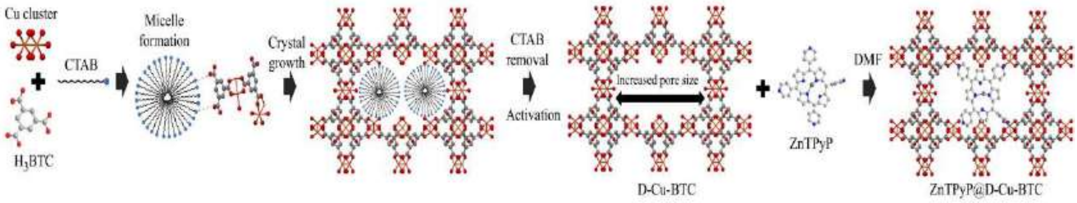
Keywords: MOFs, Defects, PSM, Loading

Incorporating active guests into metal-organic frameworks (MOFs) holds great potential for developing advanced materials with diverse applications. However, during synthesis methods often compromise MOF stability and morphology. To overcome these limitations, post-synthetic modification (PSM) offers a more controlled approach, but the inherent microporous nature of MOFs presents challenges for loading larger guests. While conventional methods for pore enlargement like ligand expansion and modulator-induced defect development have been explored, these approaches often lead to unstable structures or uncontrollable pore sizes [1]. To address these issues, we employed a surfactant self-assembly strategy using cetyltrimethylammonium bromide (CTAB) to create mesopores within the microporous Cu-BTC, resulting in a defect-engineered MOF (D-Cu-BTC) with enhanced pore size [2]. This strategy successfully resolved diffusion limitations associated with the microporous structure, as confirmed by FT-IR and BET analyses. Subsequently, Zn(II) tetrapyridylporphyrin (ZnTPyP), a macromolecule with promising applications, was post-synthetically loaded into the framework pores. UV-Vis, BET, EDX, FE-SEM, and TGA confirmed the efficient and homogenous loading of the metalloporphyrin within the modified framework structure (**Scheme 1**).



Scheme 1: Schematic illustration of surfactant-assisted pore expansion in Cu-BTC and subsequent post-synthetic loading of metalloporphyrin.

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Remediation of Alizarin Yellow from aqueous sources by Quasi-UiO-66; Box-Behncken design optimization and adsorption characterization

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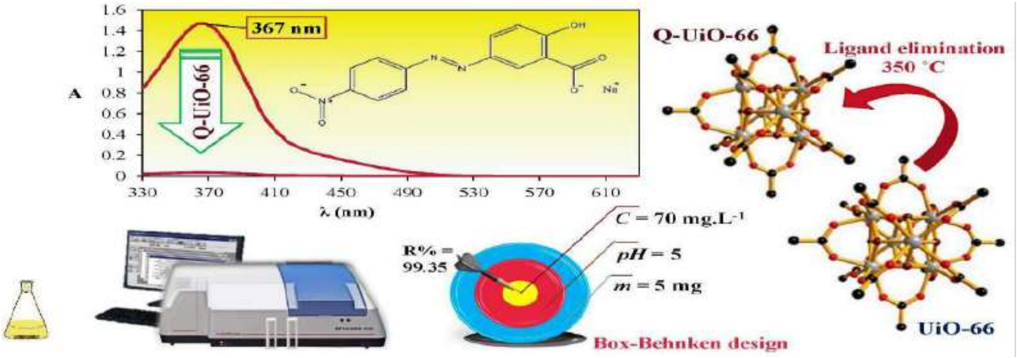
Keywords: Q-UiO-66, Alizarin Yellow, Removal

The preparation of Quasi-metal-organic frameworks (Q-MOFs) with unsaturated metal sites can effectively achieve the activity amplification of MOF based adsorbents. In this research, a modified variant of UiO-66 known as Q-UiO-66 was successfully synthesized by subjecting UiO-66 to controlled thermal partial ligand elimination at 350°C[1]. Various surface analyses, including infrared spectroscopy (FT-IR), Field emission scanning electron microscopy (FE-SEM), BET surface area analysis, X-ray diffraction (XRD) analysis, and elemental analyses, were conducted to characterize the synthesized adsorbent. To optimize the performance of remediation of the synthesized Q-UiO-66, the Box-Behnken design approach has been implemented, utilizing the principles of response surface methodology. The findings reveal an extraordinary removal of the anionic dye (AY GG), exhibiting an unprecedented uptake capacity of 398.2 mg.g^{-1}[2]. This is the first report of using a thermal ligand elimination approach to create defective UiO-66 structures with targeted pollutant removal capabilities, providing valuable insights for designing advanced MOF adsorbents[1](**Scheme1**).



Scheme 1: Remediation of Alizarin Yellow GG by Q-UiO-66

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Green synthesis of silver nanoparticles by using *Polygonum aviculare L.* extract

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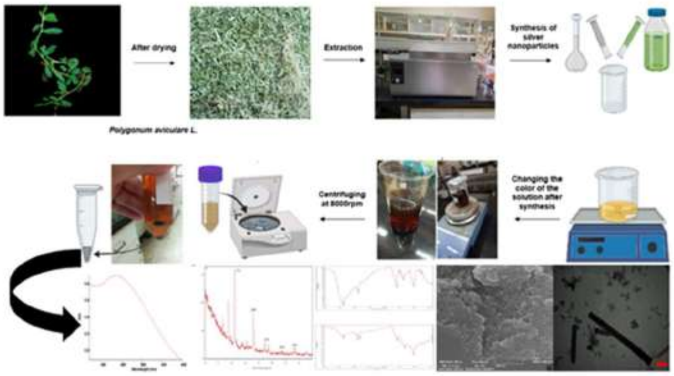
Keywords: Silver nanoparticles, Green synthesis, XRD, FESEM, *Polygonum aviculare L.*

Recent research focuses on the green synthesis of silver nanoparticles (AgNPs) using Polygonum aviculare L. extract, noted for its environmental compatibility and economic advantages. First, the polygonum aviculare L. extract was prepared by maceration and synthesized by 2 mM $AgNO_3$ solution using the green method. After changing the color of the solution, confirmation of the formation of nanoparticles by UV-Vis spectroscopy, and Morphological investigation by TEM, FE-SEM, XRD, and FT-IR to examine functional groups in nanoparticles confirmed the production of spherical and rod-shaped nanoparticles averaging 18-55 nm in size. The findings showed that Polygonum aviculare L. effectively reduces Ag+ ions to synthesize AgNPs with promising medicinal applications **(Scheme1)**.



Scheme 1: Graphical abstract of the green synthesis process of AgNPs from P. aviculare L.

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Preparation of Mg-Al LDHs and investigation the effect of temperature and solvent on nanoparticles size

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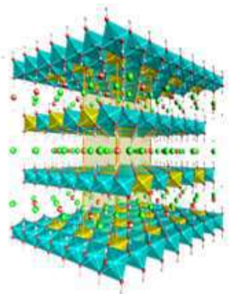
Keywords: Mg-Al, LDH, nanoparticles**,** 1-propanol

Layered double hydroxides (LDHs) are a class of nano ordered layered compounds, referred to as hydrotalcites. The general formula of LDH can be described as $[M^{II}_{1-x}M^{III}_{x}(OH)_2]^{x+}[A^{n-}_{x/n}\cdot yH_2O]^{x-}$, where M^{II} and M^{III} represent divalent and trivalent metal ions, A^{n-} is an n-valent anion (scheme 1) [1].



Scheme1: Structure of Layered double hydroxide

The properties of LDHs are controlled from their compositions (M^{2+}, M^{3+}, A^{n-} and their ratios) and morphology (particle shape, size and size distribution), making them more attractive for several applications [2]. Controlling the shape and size of the layered inorganic–organic hybrid particles is a challenge with conventional methods of synthesis. In this project, the co-precipitation method has been modified to synthesize Mg/Al Layered double hydroxide with Mg/Al molar ratio of 3:1 by controlling the particle growth under different conditions of solvent, temperature, and reaction time. All samples were characterized by X-ray powder diffraction (XRPD), and the size and morphology of nanoparticles were examined by scanning electron microscopy (SEM). The results showed that in a mixture of water and 1-propanol solvents and glycerol in the ratio of 6:1:1, temperature of 160°C and reaction time of 24 hours, nanoparticles with the highest crystallinity and the smallest size (27 nm) are obtained. According to the SEM images, LDH nanoparticles have a sheet-like shape.

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Synthesis and characterisation of nanohybrids of Cetirizine -intercalated Al–Mg layered double hydroxide

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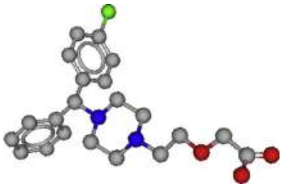
Keywords: Nanohybrid, Cetirizine, Al–Mg, layered double hydroxide

Layered double hydroxides (LDHs) or hydrotalcite-like compounds are presented by the general formula $[M^{II}_{1-x}M^{III}_{x}(OH)_2]^{x+}[A^{n-}]_{x/n}.yH_2O$. It is the possibility of varying the identity and relative proportions of the di- and trivalent cations, as well as the identity of the interlayer ions, that gives rise to the large variety of materials. On the other hand, nanomaterial-based drug delivery systems have attracted increasing attention to improve the pharmacological and therapeutic efficacy of drugs. Among the various nanoparticles, LDHs are most suitable as drug delivery carriers due to their low toxicity, high reserving capacity and enhanced cellular uptake behavior [1]. Recently, incorporation of organic anions in the interlayer space of LDHs by an ion exchange mechanism, a so-called intercalation phenomenon, was used for the synthesis of drugs and inorganic hybrid materials. Cetirizine dihydrochloride, (Scheme 1) is one of the second-generation of antihistamines, which reduces the natural chemical histamine in the body. It is used to treat cold or allergy symptoms such as sneezing, itching, watery eyes, runny nose, and other allergies, such as allergies to molds and dust mites [2,3].



Scheme 1. Molecular structure of cetirizine.

In this study, Cetirizine was intercalated into Mg–Al layered double hydroxides (LDHs) to obtain Cetirizine–LDH nanohybrids. Powder X-ray diffraction (XRD) indicates a successful intercalation of Cetirizine with a vertical orientation. Intercalation of organic anion of Cetirizine into Mg–Al LDH caused the interlayer spacing of LDH to increase from 0.88 to 2.52 nm as determined by XRD studies.

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Fabrication of polymer nanocomposite with apricot tree gum decorated with magnetite nanoparticles to absorb electromagnetic waves

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Keywords: Electromagnetic waves, Magnetite, Gum, Reflection loss

Recent advances in electronic devices have greatly improved our daily lives. However, the abundant presence of electromagnetic radiation from these devices has caused ecosystem pollution [1]. Therefore, there is a need to develop materials with the capacity to absorb electromagnetic waves that can reduce electromagnetic radiation pollution [2-4]. In this work, spinel iron oxide is used to induce high magnetic losses. Magnetite nanoparticles (Fe_3O_4) show a high surface-to-volume ratio, however, some drawbacks such as high mass density and limited dielectric losses need to be overcome. With this in mind, the natural polymeric apricot tree gum was decorated with Fe_3O_4 nanoparticles. For this purpose, apricot tree gum (R) was soaked in deionized water. The resulting solution was kept at room temperature for 24 h. The gum solution was added to the metal salt solution under magnetic stirring and the temperature of the combined solution was increased to 80°C. After 15 min, NaOH was added to the solution and finally, the precipitate was separated by a magnet. The morphology of Fe_3O_4/R nanocomposite was investigated using FESEM, the Fe_3O_4 nanoparticles with spherical structures are well dispersed in the apricot tree gum matrix, and as a result, a uniform morphology of the composite is created. The Bragg reflections obtained from the magnetic nanocomposite from the X-ray diffraction pattern prove that the ferrite nanoparticles obtained by this method have a spinel cubic structure (ICDD Card No. 01-088-0315). The average crystal size of Fe_3O_4 nanoparticles in the composite was calculated to be 10.3 (±0.8) nm. A vector network analyzer (VNA) was used to analyze the electromagnetic parameters of the samples, using a WR90 waveguide in the range of 8-12 GHz. Reflection loss (RL) of Fe_3O_4/R nanocomposite RL=-71.09 dB occurs at 10.45 GHz frequency for 1 mm thickness. This nanocomposite shows the highest reflection losses and covers the entire X-band.

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Photocatalytic Degradation of Tetracycline over Al_2O_3/CuO Carbon Doped Composites Derived, from in-Situ Carbonization of Al(FUM)

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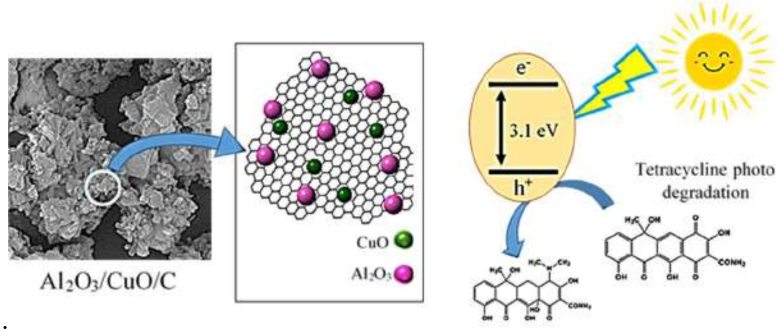
Keywords: Metal organic frameworks, Degradation, Carbon doped materials and photocatalytic

The improper disposal of antibiotics, such as tetracycline [2], leads to environmental contamination and poses significant health risks [1-3]. Effective remediation strategies are crucial [4]. In this study, we synthesized Al_2O_3/CuO carbon-doped composites through a multi-step process involving the in-situ carbonization of aluminum fumarate (Al(FUM)) (**Scheme1)**. The synthesis began with the preparation of Al(FUM), followed by the adsorption of copper metal ions (Cu^{2+}) onto the Al(FUM) framework. This was achieved by immersing the Al(FUM) in a copper precursor solution, allowing Cu^{2+} ions to be incorporated into the framework. Subsequently, pyrolysis was performed on the Cu-loaded Al(FUM) to form the Al_2O_3/CuO composite with carbon doping. The resultant Al_2O_3/CuO/C composites were characterized using XRD, SEM, FT-IR, UV–Vis DRS, N_2 adsorption–desorption isotherms, XPS, and EIS to confirm their structural and physicochemical properties. The photocatalytic performance of these composites was evaluated for the degradation of tetracycline hydrochloride under simulated sunlight. The Al_2O_3/CuO/C composite demonstrated exceptional photocatalytic activity, achieving a rapid degradation rate with a significant rate constant. The primary active species responsible for the degradation was identified as $\cdot O_2^-$, and the degradation mechanism was determined to follow a type II heterojunction photocatalytic reaction. This study provides a novel approach for designing high-efficiency photocatalysts and offers insights into the degradation of other organic pollutants.



Scheme1: synthesis plan for preparation of Al_2O_3/CuO/C

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A Simple Method for Validation Hydroquinone in Liposomal Matrix

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Keywords: Hydroquinone, Liposome, UV Spectroscopy, Validation

In determining the concentration of a molecule, a method should be used that does not interfere with other molecules in the matrix [1]. In pharmacy, where a drug is formulated in different forms, it is necessary to validate the method of determining the concentration in the desired matrix [2]. In this study, a simple method was used to determine the concentration of hydroquinone in the liposomal matrix. The samples were dissolved in methanol and evaluated in 293 nm by UV spectrophotpmetery. The validation parameters such as linearity, accuracy, precision, specificity, limit of detection (LOD) and limit of quantization (LOQ) were determined. The calibration curve was linear in 1-50 µg /mL range of hydroquinone analyte with a regression coefficient of 0.9998. This study showed that the liposomal hydroquinone composed of phospholipid (7.8 %), cholesterol (1.5 %), alpha ketopherol (0.17 %) and hydroquinone (0.5 %) did not absorb wavelength of 293 nm if it diluted 500 times by methanol. The concentration of hydroquinone reached 10 µg /mL after 500 times of dilution. Furthermore, various validation parameters as per ICH Q2B guideline [3] were tested and found accordingly. The recovery percentages of liposomal hydroquinone were found 102±0.8, 99±0.2 and 98±0.4 for 80%, 100% and 120% respectively. The relative standard deviation values of inter-day precision and intra-day precision were <%2. LOD and LOQ were 0.24 and 0.72 respectively. With a simple UV spectrophotometric method, the concentration of hydroquinone in the liposomal formulation was measured

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Introducing Novel Carbene Ligands with Electronic Stabilization and Innovative Catalytic Applications

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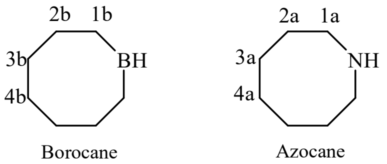
Keywords: Carbene Ligands, Borocane, Azocane, DFT Calculations, Catalysis

Carbenes are highly reactive species consisting of a carbon atom with two unpaired electrons. They exist in two states: singlet and triplet, as shown in Scheme 1. In the singlet state, the electrons are paired in one orbital, aiding in new bond formation, while in the triplet state, the electrons occupy different orbitals, leading to increased stability. These compounds serve as crucial intermediates in chemical reactions and complex syntheses. [1].

Scheme 1: Structure of carbene in singlet and triplet states

This study introduces carbene derivatives of azocane (NH) [2] and borocane (BH) [3], focusing on eight isomers 1a-4a and **1b-4b** (Scheme 2). Using DFT calculations at the B3LYP/6-311+G* level via Gaussian software, the stability of singlet and triplet states was evaluated. The analysis reveals that certain isomers exhibit enhanced stability due to resonance (**1a, 1b**) or the formation of a stable five-membered ring (**4a, 4b**). Isomers **1a** and **4a** are 64.3 and 30.8 *kcal.mol*$^{-1}$ more stable than their non-heteroatom counterparts, while isomers **1b** and **4b** are 22.1 and 15.7 *kcal.mol*$^{-1}$ more stable. These derivatives, with their unique electronic properties, are promising candidates as ligands in metal complexes and innovative catalysts, particularly in hydrogenation, cross-coupling, and polymerization reactions.



Scheme 2: Eight Different Carbene Isomers of Azocane and Borocane

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Enhanced Oxidation of Benzyl Alcohol Using Mixed Metal PCN-250 Catalyst

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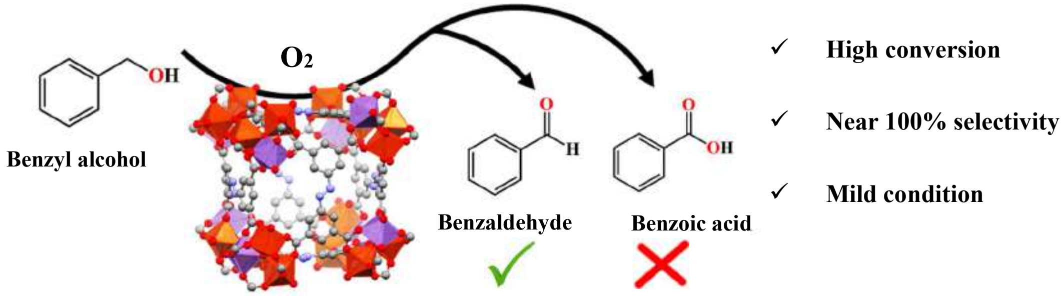
Keywords: MOF, Benzyl alcohol, Catalysis, Oxidation, MOF Cluster

The development of novel metal-organic frameworks (MOFs) has garnered significant attention due to their versatile applications in catalysis, gas storage, and separation [1]. In this study, we report the synthesis and characterization of a mixed metal (Fe and Mn) cluster PCN-250 [2]. This MOF was designed to perform the catalytic oxidation of benzyl alcohol to benzaldehyde.

The synthesis of the mixed metal PCN-250 was achieved through a solvothermal method, utilizing iron and manganese precursors in the presence of a 3,3’,5,5’-azobenzenetetracarboxylic acid linker. The resulting material was thoroughly characterized using various techniques. XRD, XPS, EPR, ICP and FTIR spectroscopy [3].

The catalytic performance of the synthesized PCN-250 was evaluated in the oxidation of benzyl alcohol to benzaldehyde. The results demonstrated high conversion and selectivity of benzaldehyde over benzoic acid [4]. These findings highlight the potential of the mixed metal PCN-250 as an efficient catalyst for selective oxidation reactions, paving the way for further exploration of its applications in other catalytic processes.



Scheme1: Mixed metal Fe/Mn cluster PCN-250 as catalyst in oxidation of benzyl alcohol.

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Solvent-Free CO_2 Fixation with PCN-250(Fe): role of Trimetallic Clusters

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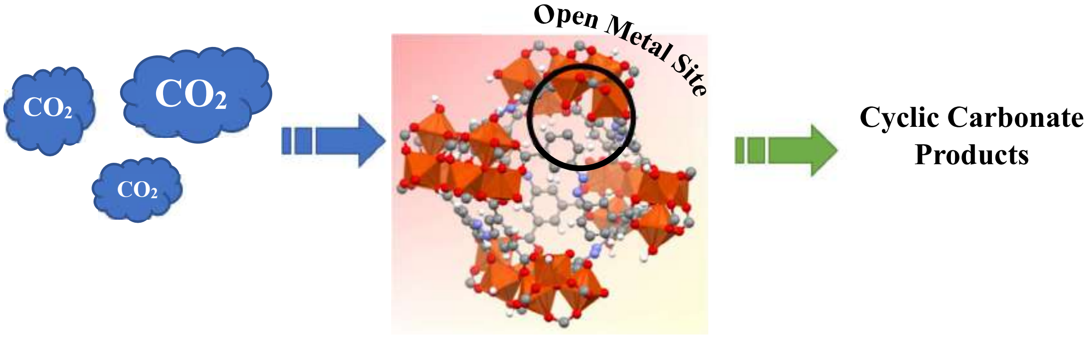
Keywords: MOF, CO_2 fixation, Catalysis, Defective MOF, Environment

CO_2 fixation is a crucial process in addressing environmental challenges by converting CO_2 into valuable chemicals. [1] One promising approach is the transformation of styrene oxide into 5-membered cyclic carbonate, which can be achieved under solvent-free conditions, offering a sustainable and efficient method for CO_2 utilization. [2]

In this study, PCN-250(Fe) was synthesized using of 3,3',5,5'-azobenzenetetracarboxylic acid as linkers. The synthesis involved solvothermal conditions, resulting in a robust MOF with high surface area and active metal sites suitable for catalytic applications. In order to evaluate structural details a set of analysis including XRD, BET, FTIR, XPS, SEM, etc. were conducted. [3] The catalytic performance of PCN-250(Fe) in the CO_2 fixation reaction of styrene oxide demonstrated remarkable efficiency, achieving over 90% conversion to cyclic carbonate in less than 2 hours. This highlights the potential of PCN-250(Fe) as an effective catalyst for sustainable CO_2 utilization.



Scheme1: CO_2 fixation reaction via PCN-250 with Fe open metal sites.

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Breathing Effect of MIL-53(Al) in Sensing Nitroaromatic Compounds

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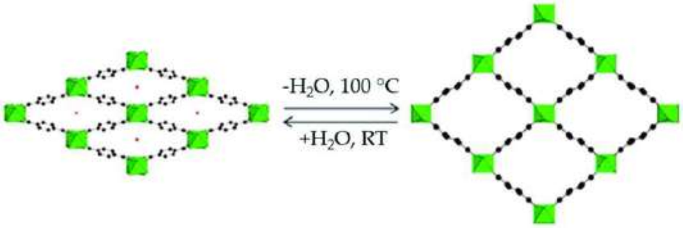
Keywords: MIL-53(Al), Breathing effect, Sensing, Nitroaromatic compounds

MIL-53(Al) is known for its unique breathing effect, which allows it to transition between closed and open pore structures depending on the presence or absence of water molecules (which is known as breathing effect), makes it particularly interesting for sensing applications, as it can dynamically respond to environmental changes. The framework's ability to switch between different pore structures enhances its potential for detecting various compounds, including nitroaromatic compounds. [1]

In this study, MIL-53(Al) was synthesized via solvothermal method and its breathing effect was explored for sensing nitroaromatic compounds. Various analytical techniques were employed to characterize the material, including FTIR, UV-Vis, PL spectroscopy and BET analysis. These techniques provided comprehensive insights into the structural and functional properties of MIL-53(Al). [2]

The sensory applications of MIL-53(Al) were evaluated by investigating its ability to detect nitroaromatic compounds in acetonitrile solvent. The results revealed that the open pore structure, form stronger interactions with analyte with the highest sensing for TNT. In contrast, nitrophenol showed superior sensing capability in the narrow pore structure. These findings underscore the potential of MIL-53(Al) as a versatile sensor for nitroaromatic compounds under varying environmental conditions.



Scheme1: Figure 1: breathing effect of the MIL-53(Al) [3].

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Zn-based metal-organic framework for oxygen evolution reaction application

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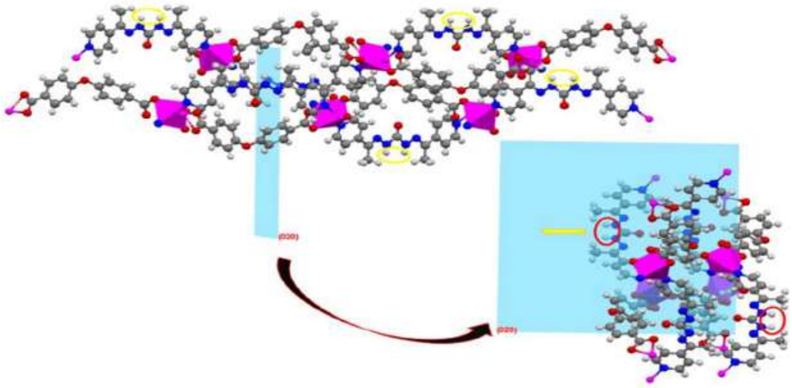
Keywords: Pillar MOF, OER, Conductivity, Energy conversion

electrocatalytic overall water splitting (OWS) consists of two half-cell electrode reactions, the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER), occurring on the anode and cathode, respectively. the OER due to the sluggish four-electron transfer needs to consume large electric energy to overcome the reaction energy barrier [1].

In this study, pillared MOF TMU-58 was synthesized via previous methods [2], and then deposited into nickel foam (NF) for investigation of the oxygen evolution reaction (OER) procedure. TMU-58 exhibits a low overpotential of 256 mV at a current density of 10 mA cm^{-2} which is attributed to the pillar linker in the structure that facilitate charge transfer and boosts OER activity.



Scheme 1. Structure of pillared metal-organic framework TMU-58

References

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Vanadium Complexes with Tetradentate Schiff base: Synthesis, Characterization and Biological activity

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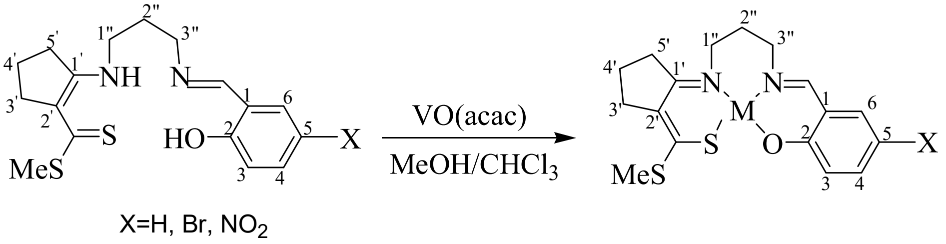
Keywords: Schiff bases, Vanadium complexes, Spectroscopic data, Antibacterial.

The oxidovanadium(IV) complexes have attracted considerable interest in drug discovery due to the development of their medicinal applications [1]. In particular, vanadium compounds show insulin mimetic activity, were tested in clinical trials [2]. Vanadium complexes with Schiff base ligands have a great deal of attention all this affects their biological activity. Three new oxidovanadium (IV) complexes with unsymmetrical Schiff base ligands were synthesized and characterized by various spectral techniques were used to confirm the structures. It has been found that the Schiff base behaves as a tetradentate ligand forming chelates with 1:1 metal:ligand stoichiometry. The coordination sphere of each V atom constructed from four donor atoms of the ligand with NNOS donor sites and one oxido oxygen. Antibacterial activities of the prepared compounds were evaluated in vitro against S. Aureus and E. Coli. The ligands and their complexes exhibited significant antibacterial activity. The free ligands showed high activities compared with the VO^{IV} complexes.



Scheme1: Synthesis of oxidovanadium(IV) complexes.

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In Situ Single-Crystal-to-Single-Crystal Structural Transformation in Dynamic Coordination Networks

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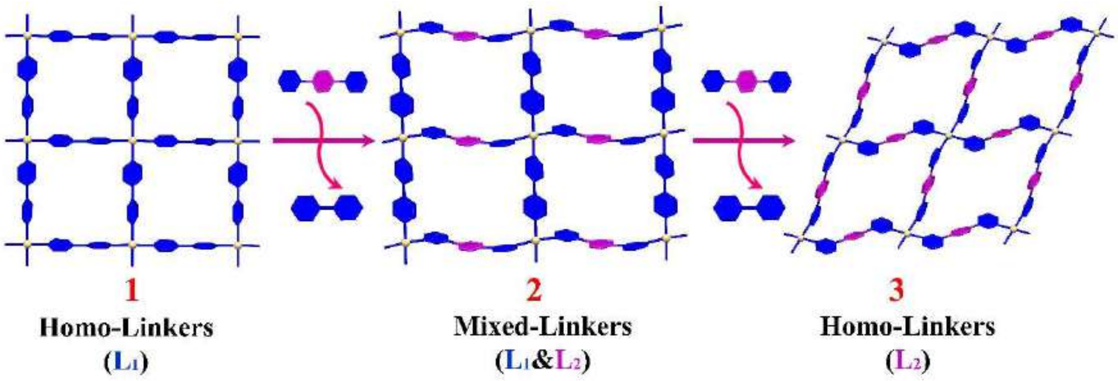
Keywords: Structural transformation, Core@shell crystals, Linker replacement, Coordination network

In recent two decades, coordination polymers and coordination networks have attracted extensive attention as one of the most significant categories of designable materials with attractive and adjustable structural properties.[1, 2] In current study, we reported a case of rare *in situ* linker replacement in cadmium coordination networks based on L_1 and L_2 through single-crystal-to-single-crystal (SC-SC) structural transformation manner. In the first step, 2D homo-linkers coordination network of $\{[Cd(L_1)_2(ClO_4)_2](CHCl_3)_4\}_n$ (1) transformed into 2D mixed-linkers coordination network of $\{[Cd(L_1)(L_2)(ClO_4)_2](CHCl_3)(MeOH)\}_n$ (2) via core@shell crystal and SC-SC structural transformation process after two weeks. In the second step, standing coordination network of 2 in mother mixture, leads to SC-SC structural transformation to 2D rhombic-grid homo-linkers of $\{[Cd(L_2)_2(H_2O)_{1.4}(MeOH)_{0.6}](3,3'\text{-pytz})(MeOH)_{1.4}(ClO_4)_2\}_n$ (3) after two months (**Scheme 1**).



Scheme 1: Facile and *in situ* linker replacement in cadmium coordination networks.

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Electrochemical Fabrication of Cu-Doped ZnO Nanoparticles and Investigation of Their Photocatalytic Properties

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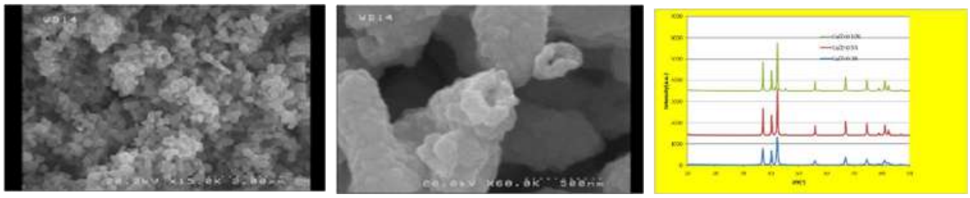
Keywords: Electrochemical method, Nano metal Oxide, Photocatalytic properties

Over the last decade, nanostructures have attracted special attention due to their unique properties, such as high surface area, excellent penetration, and distinct optical characteristics. These properties have led to significant applications in various fields, including catalysis, fillers, coatings, chemical storage, pigments, artificial cells, and the protection of light-sensitive components [1]. In this work, Cu-doped zinc oxide nanoparticles with a high surface area were prepared using an electrochemical method under normal conditions of temperature, pressure, and environment in the presence of air [2,3]. Products were characterized using Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), field scanning electron microscopy (FSEM), and UV-visible spectrophotometry (UV) (Figure 1, a, b, and c). The Cu/ZnO nanoparticles were studied to evaluate and compare their photocatalytic activity, particularly in the degradation of methylene blue dye. The results showed that the photocatalytic activity of Cu-doped zinc oxide nanoparticles prepared using the electrochemical method has improved compared to other methods of preparing Cu/ZnO nanoparticles.



(a) (b) **(c)**

Scheme1:(a) and (b), Scanning electron microscope image (SEM) of the Cu/ZnO nanoparticle, (C), XRD diffraction pattern for nanostructures of Cu/ZnO nanoparticle(3-10%).

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New Schiff base and its mercury pseudo halide Complex: Synthesis, Characterization, Thermal and Biological Properties

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Keywords: Schiff base, Mercury Complexes, Thermal and Biological Study.

Schiff base and their structural analogues as ligating compounds containing imine C=N bonds, are of great importance in modern chemistry. The long chain ligands have been derived from condensation reaction between carbonyls and diamines. Recently imino-organic compounds and their metal complexes have received attention due to their biological properties, chemo-sensors and industrial applications. Among metal Schiff base complexes, the mercury complexes especially with coordinated pseudo halide are rare. Although, the metallic and some mercury salts are toxic but some organomercury compounds have been proved to have useful and unique biological activity [1- 3].

In continuation of other reports on synthesis and biological applications, in this research, some pseudo halide mercury complexes with a new Schiff base ligand (bis(methoxyphenylallylidene)-propanediamine) have been prepared and characterized by various spectroscopic techniques. General formula suggested of these complexes is $[HgLX_2]$ (X is pseudohalide). The synthesized Schiff base compounds were screened *in vitro* for their antimicrobial activity against various fungi and bacteria. These new complexes show antifungal and antibacterial properties. Furthermore, the thermal behavior and some thermo-kinetic activation parameters such as (E*), (ΔH*), (ΔS*) and (ΔG*) were established by TG/DTG/DTA curves.

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In silico studies of mono- and di-nuclear metal complexes of curcumin-nicotinoyl

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Keywords: Metal complexes of curcumin-nicotinoyl, Bioactivity prediction, Molecular docking

Curcumin-nicotinoyl (Cur-Nic) was used as a ligand for the synthesis of mono- and di-nuclear copper(II) and zinc(II) complexes [1]. As the tyrosine-protein kinase SRC (abbreviated as SRC) is one of the proteins activated abnormally in several malignancies [2], the docking studies of Cur-Nic and its metal complexes with SRC were performed using PyRx software. The results of the docking studies indicate the binding affinity of -9.1, -10.0, -9.4, -11.8, and -3.0 kcal/mol to the tyrosine-protein kinase SRC for Cur-Nic, mono-nuclear Cu(II) complex, di-nuclear Cu(II) complex, mono-nuclear Zn(II) complex, and di-nuclear Zn(II) complex, respectively. Consequently, metal complexes bind to SRC stronger than Cur-Nic except for di-nuclear Zn(II) complex. Consequently, the order of effectiveness of each compound on the SRC is mono-nuclear Zn(II) complex > mono-nuclear Cu(II) complex > di-nuclear Cu(II) complex > Cur-Nic > di-nuclear Zn(II) complex. According to **Table 1**, the number of amino acids involved in hydrogen bonds with the compounds is higher for di-nuclear complexes than others. Higher coordination potential of these complexes contributes to the mode of binding to the SRC.

Table 4 Amino acids involved in hydrogen bonds with the compounds based on docking results**.**

Compound	Amino acids involved in hydrogen bond
Cur-Nic	LYS295A-ASP404A-ARG388A-CYS277A
Mono-nuclear Cu(II) complex	SER345A-ARG388A-TYR340A-GLU353A
Di-nuclear Cu(II) complex	CYS27A-LYS295A-GY279A-GLN275A-PHE278A-MET341A-SER345-ARG388A
Mono-nuclear Zn(II) complex	ARG388A-LEU273A- THR338A
Di-nuclear Zn(II) complex	ALA390A-CYS277A-LYS295A-PHE278A-TYR416A-ARG288A-GLN275A-ASP348A-SER345A

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C−S Cross-Coupling Reaction of Thiols and Arylboronic Acid in the Presence of Copper(II)-Terpyridine Complexe

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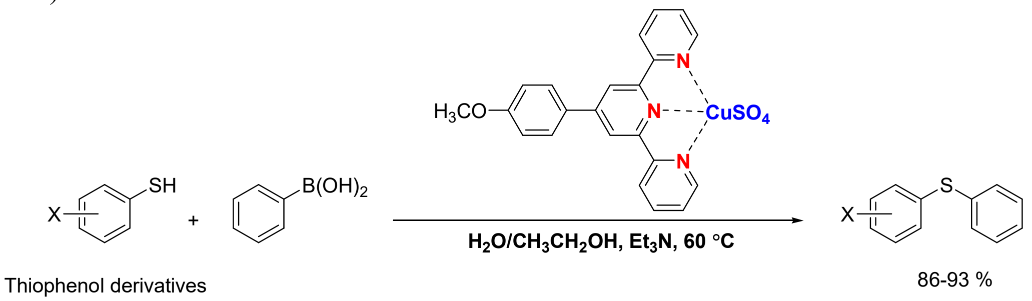
Keywords: C−S Cross-Coupling Reaction, Aryl Thioethers, Copper-Catalyzed Reaction, Arylboronic Acid, Thiol

In recent years, the C–S cross-coupling reaction has become a crucial research area in modern organic chemistry due to the various applications of aryl thioethers in various fields such as biology, medicine, agriculture, and materials science.[1] Although some progress has been made, considerable attention is still being paid to the development of new catalyst systems to improve the transition metal catalyzed C–S cross-coupling reaction.[2] Since the leachability of transition metal catalysts is a key factor in catalytic processes, the design and/or use of organic ligands with carefully placed binding sites offers great potential for the fabrication of novel structural complexes. Therefore, the use of electron-rich ligands to anchor transition metals is an important factor. In this regard, to identify a potent and readily prepared system for catalyzing C–S cross-coupling reaction, we utilized 4′-(4-methoxyphenyl)-2,2′:6′,2″-terpyridine ligand and $CuSO_4$ in investigating its effectiveness in C–S cross-coupling reaction. The use of a simple, electron-rich terpyridine tridentate ligand will prevent any leaching of the copper active sites, resulting in a very stable complex and a more effective catalytic system (**Scheme1**).



Scheme1: Displaying the effectiveness of our catalytic system in the Cu-catalyzed C–S cross-coupling reaction.

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Synthesis and application of $PbCO_3$/rGO nanocomposite for enhanced performance in lead-acid batteries

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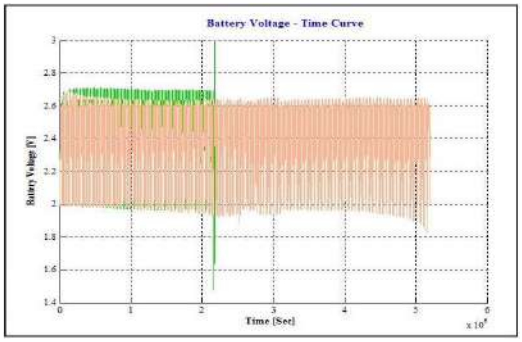
Keywords: Lead- acid battery, Graphene oxide, Pb, Nano composite

The lead-acid battery, with a history spanning over 150 years, remains the oldest rechargeable battery technology [1]. However, these batteries face significant challenges, including low energy-to-volume ratio, low energy-to-weight ratio, limited cycle life under partial charge conditions at high rates, and sulfation [2]. In this study, a $PbCO_3$/rGO nanocomposite has been utilized to inhibit sulfation and extend the charge-discharge cycle life of the battery cell. This nanocomposite was synthesized in-situ by the hydrothermal method at a temperature of 180°C. $PbCO_3$/rGO nanocomposite was used as an additive in the active material of the negative electrode at the rate of 1% by weight to prevent sulfation of the lead-acid battery. The lifetime of the battery cell containing the $PbCO_3$/rGO nanocomposite increased 2.5 times compared to the battery cell without this nanocomposite. The charge transfer resistance and ion exchange resistance in the cell containing $PbCO_3$/rGO nanocomposite decreased, and the sulfation of the negative electrode was also delayed.The result shows that graphene oxide nanocomposite containing lead in the negative electrode of lead-acid battery can significantly improve its performance.



Scheme: The graph of battery voltage versus time is shown for the normal lead-acid battery cell sample in light green color and the PbCO3/rGO nanocomposite battery cell sample in orange color.

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Cadmium halide Complexes: biological, thermal and theoretical investigation

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Keywords: Cadmium complexes, Schiff base, Theoretical, Thermal and Biological Study.

Nowadays, Schiff base compounds as an important class of ligands are of great interest in coordination chemistry due to their flexibility, easily preparation and diversity of their properties. Recently various cadmium Schiff base complexes have been synthesized and subjected to *in vitro* biological screening [1-3]. In continuation of other researches on this topic, herein, some halide cadmium complexes with a new Schiff base ligand (bis(3(2-methoxyphenyl)-1-propenaldehyde)-propanediimine) have been prepared and characterized by physical and spectral methods. Moreover the compounds were screened *in vitro* for their antimicrobial activity against various fungi and bacteria (fig.1). These new complexes show antifungal and antibacterial properties. Furthermore, some thermo-kinetic activation parameters such as (E*), (ΔH*), (ΔS*) and (ΔG*) were evaluated by TG/DTG/DTA curves. Finally, the structural geometry of the compounds was theoretically investigated by DFT method.

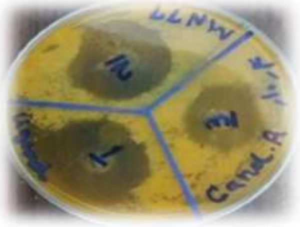

Fig.1. Antifungal activity of the ligand against C. *albicans* and A. *niger.*

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Synthesis, spectral characterization, theoretical and thermal study of two new biological active Zinc(II) azide and thiocyanate complexes

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Keywords: Zinc complexes, Schiff base, Theoretical, Thermal and Biological Study.

Nowadays, imine compounds are important class of ligands in coordination point of view. Some applications of the iminic compounds and their zinc complexes are antimicrobial, antiviral, anticancer, anti-inflammatory and anticorrosion activities. [1-3]. Herein, two new zinc complexes with a new Schiff base ligand (bis(3(methoxyphenyl)-1-propenaldehyde)-hexanediimine) have been prepared and characterized by physical and spectral(IR and NMR) techniques(fig.1). Moreover the complexes were checked *in vitro* for their antibacterial/antifungal activities against various fungi and bacteria. These new zinc complexes showed considerable antifungal and antibacterial properties. Furthermore, some thermo-kinetic activation parameters such as (E*), (ΔH*), (ΔS*) and (ΔG*) were evaluated by TG/DTG/DTA curves. Finally, the structural geometry of the complexes was theoretically investigated by DFT method.

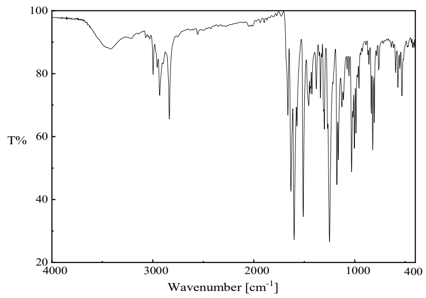

Fig.1. FT/IR spectrum of the ligand.

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Some new cadmium pseudohalide complexes: preparation, theoretical, thermal stability and antibacterial/antifungal bioassay

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Keywords: cadmium complexes, Schiff base, Theoretical, Thermal and Biological Study.

Schiff base ligands introduce potential active sites for biochemical activities against various pathogen microorganisms. Moreover, cadmium complexes of Schiff base ligands exhibit a variety of properties in biological, analytical, clinical and industrial points of view [1-3].

In this work, two new pseudohalide cadmium complexes with a new Schiff base ligand (bis(3(*o*-methoxyphenyl)-1-propenaldehyde)-1,2-propanediimine) have been synthesized and identified by some physical and spectral techniques. Moreover the complexes were checked *in vitro* for their antibacterial/antifungal activities against various microbes. These new cadmium complexes exhibited notable antimicrobial activities. Furthermore, some thermo-kinetic activation parameters such as (E*), (ΔH*), (ΔS*) and (ΔG*) were calculated using Coats-Redfern relationship based on TG/DTG/DTA diagram(fig.1). At final, DFT calculation method was applied to investigate theoretically the structural geometry of the complexes.

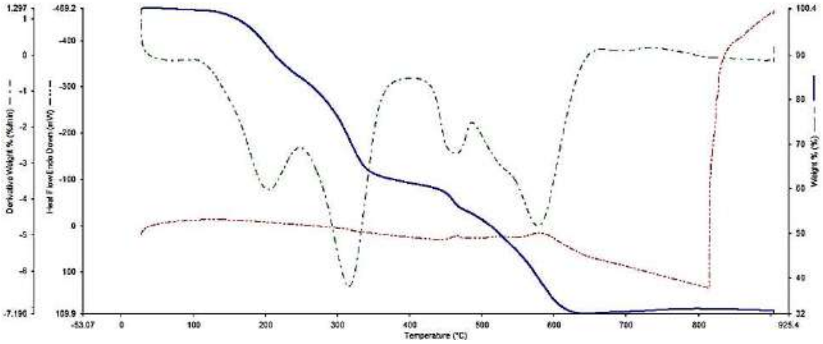

Fig. 1. TG/DTG/DTA diagrams of cadmium thiocyanate complex.

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An Effective Polyoxometalate- Ionic Liquid Heterogeneous Catalyst to Desulfurization

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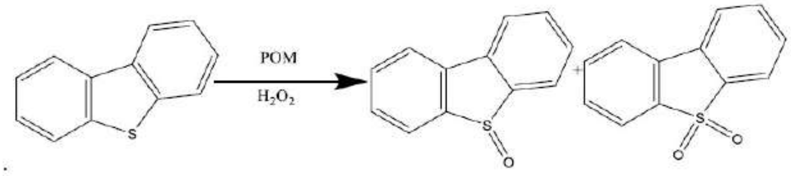
Keywords: Oxidation; Desulfurization; Polyoxometalates, H_2O_2

Recently, air pollution as a global problem is a basic concern of the world. For this reason, the reduction of air pollution in the world for environmental conservation has attracted massive research interest and promoted the research demand of optimizing deep desulfurization technologies. Developing desulfurization catalysts with high activity has been one of the most important subjects [1]. Aromatic organosulfur compounds, as one of the main pollutant sources, widely exist in liquid fuel, and the sulfur oxides produced by fuel combusting are the main source of environmental pollution [2]. Oxidative desulfurization (ODS) has been highlighted as a promising complementary or alternative method since high efficiency can be achieved under mild reaction conditions [3]. A polyoxometalate-based frameworks ionic liquid (Hexadecyltrimethylammonium chloride) composite $(HTEC)_5[W_{12}CoO_{40}]._3H2O$ has been prepared as effective and reusable heterogeneous catalysts for the selective oxidation of Dibenzothiophene (DBT) by hydrogen peroxide as a green oxidant. DBT were oxidized to the corresponding sulfone and sulfoxide with excellent conversion. Our results showed that the ionic liquid-polyoxometalate was stable to leaching, behaved as true heterogeneous catalysts, were easily recovered by filtration, and reused three times with the maintenance of the catalytic performance (**Scheme1**).



Scheme1: Desulfurize oxidative catalytic processes of DBT.

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Additive-Induced Controllable Supramolecular Isomerism in Zn(II) Coordination Polymers

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Keywords: Coordination polymer, Supramolecular isomer, Polymorph, Additive

Additive molecules can play a crucial role in the formation of supramolecular isomers. There are several examples of conformational isomers where different additives significantly influence the conformation of the ligands and the overall topology of the structures [1, 2]. However, additive-induced polymorphism in coordination polymers has been rarely reported [3]. According to Scheme 1, the polymorphs namely; $\{[Zn(4bpu)(OAc)_2](CH_3OH)\}_n$ **(1)**, $\{[Zn(4bpu)(OAc)_2](CH_3OH)\}_n$ **(2)**, and $\{[Zn_3(4bpu)_3(OAc)_6](CH_3OH)_2\}_n$ **(3)** were prepared from $Zn(OAc)_2{\cdot}2H_2O$ and the 4bpu ligand in methanol without any additive and in the presence of 3-nitrophenol and 1,3-dinitrobenzene at room temperature, respectively. Both compounds **1** and **2** have the same formula, differing only in their supramolecular interactions with each other, and they exhibit a 1D zigzag chain structure. By changing the additive, compound **3** is formed, which is characterized as 1D triple-stranded ladder structural motif. Interestingly, although these additives do not participate in the structural frameworks, it is not possible to obtain products **2** and **3** without the addition of additives.

Scheme1: Synthetic method and structural motifs for **1-3**.

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Triphenylamine-Based Hole Transporting Materials for Highly Efficient Perovskite Solar Cells

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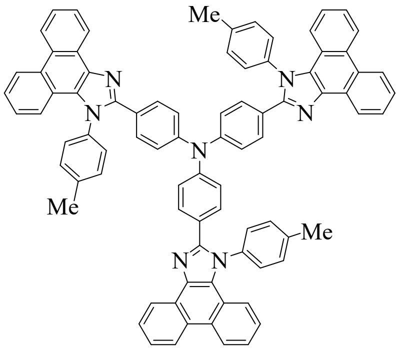
Keywords: Perovskite, Solar Cells, Hole Transporting Materials, Triphenylamine, Imidazole

Photovoltaic solar cells based on perovskites have come to the forefront in science by achieving exceptional power conversion efficiencies (PCEs) in less than a decade of research [1]. Nowadays hole-transporting materials (HTMs) based on conductive small organic molecules have become the hottest topic in high-performance perovskite solar cells (PSCs) [2]. Star-shaped triphenylamine-phenanthreneimidazole (TPA-PIM)-based HTM has been obtained through a facile synthetic route by crosslinking phenanthreneimidazole-based donor group with a triphenylamine core (**Scheme1**). The incorporation of this HTM in photovoltaic devices leads to PCE up to 17 %, thus paving the way to very efficient and highly versatile materials for light-energy conversion.



Scheme1: Structure of TPA-PIM.

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DNA interaction and cytotoxic investigations of cyclometalated platinum(II) complexes with bisphosphine ligands

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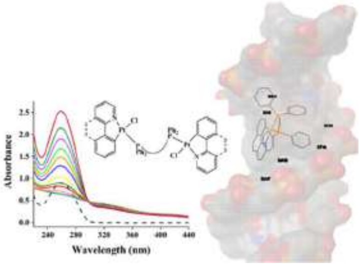
Keywords: Platinum complex, UV-vis, Fluorescence, DNA interaction, Cytotoxic activities

A series of cyclometalated platinum (II) complexes including [bhq-Pt-dppm] Cl **(C1)**, [bhq-Pt-dppa] Cl **(C2)**, [Pt$_2$-Cl$_2$-(ppy)$_2$-(μ-dppm)] **(D1)** & [Pt$_2$-Cl$_2$-(bhq)$_2$-(μ-dppa)] **(D2)** which ppy, dppm, dppa, and bhq are 2-phenylpyridinate, bis(diphenylphosphino)methane, bis(diphenylphosphino)amine, and benzo[h]quinolinate, respectively prepared as reported in literature **[1]**. To study the interaction mode and binding properties of these platinum (II) complexes with CT-DNA, UV-vis absorption, luminescence quenching techniques, and molecular docking modelling were used. The results of these studies, such as the hyperchromic effect, binding constant values (Kb), fluorescence quenching studies (incomplete quenching), and Stern-Volmer quenching (KSV) values, all indicate partial intercalation as the main interaction of these compounds with CT-DNA. Then, we investigated cytotoxic effects of all four classes of Pt complex by MTT test as a colorimetric assay for assessing cell metabolic activity on the MCF-7 breast cancer, K562 and Jurkat leukemia cell lines **[2]**. The results of the structure-activity relationship study showed that the monomeric complexes **C1** and **C2** exhibited stronger anti-tumor activity compared to the dimeric complexes **D1** and **D2**.



Scheme1: Interaction between cyclometalated platinum (II) complexes & CT-DNA.

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Synthesis and Characterization of Sulphur containing Mixed-Linker MOF-801 for Enhanced Iron Removal from Water

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Keywords: MOF, Metal ion removal, Mixed linker MOF, Environment

The removal of iron from water is a critical environmental challenge due to its adverse effects on human health and ecosystems. Metal-Organic Frameworks (MOFs), which are crystalline materials composed of metallic clusters and organic ligands, have emerged as promising adsorbents for various applications, including catalysis, gas storage, and drug delivery. Their high surface areas and tunable pore structures make them particularly effective for metal ion removal from water. [1] This study focuses on the synthesis and characterization of a novel mixed-linker MOF, incorporating sulphur containing secondary ligand into the structure of Zr-MOF, to enhance its iron adsorption capacity.

In this research, Zr-MOF was synthesized using a solvothermal method, while a secondary sulphur containing linker incorporated as precursors. The mixed-linker strategy aimed to improve the MOF's affinity for iron ions. [2] Various characterization techniques were employed to confirm the successful synthesis and structural integrity of the new MOF. XRD, BET, NMR, SEM analysis and FTIR spectroscopy identified functional groups. [3]

The results demonstrated that the introduction of the secondary linker significantly enhanced the MOF's iron adsorption capacity. The new mixed-linker MOF exhibited superior performance in selectively removing Fe ions from water up to 80% removal. The results indicate that compared to the original MOF-801, the mixed linker MOF exhibits superior metal ion removal. This research highlights the potential of mixed-linker MOFs in addressing environmental issues related to metal ion contamination, offering a promising solution for water purification and environmental remediation.

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Comparison of effect different Zeolite as a seed in Synthesis of SAPO-34 on MTO Catalytic Performance

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Keywords: Seed, SAPO-34, SAPO-`18, ZSM-5, Methanol to olefins

Hierarchical silicoaluminophosphate zeolites SAPO-34/18, SAPO-34/ZSM-5 and SAPO-34 were synthesized by adding different amounts of SAPO-18, ZSM-5 or SAPO-34 seed crystals to SAPO-34 zeolite precursor [1]. Hydrothermal system in which the addition of seed along with the reduction of the amount of template reduces the price of the synthetic catalyst. The prepared samples were characterized by XRD, FESEM, EDS, N2 adsorption-desorption, NH3-TPD. The X-ray diffraction results showed that up to 5% of the seeds in the molar ratio of template to alumina equal to 1.3 in all catalysts, the SAPO-34 without impurities synthesised. When the number of seeds in synthetic gel increased to 7%, the crystal size, impurities, and defects in the structure increased. These samples had a higher external surface and mesopore volume than the normal SAPO-34. The results of NH3 -TPD showed that the amount and strength of strong acid sites increases in samples affected by the amount of seed crystals. By increasing the SAPO-34 seed to 7%, the lifetime of the catalyst reaches 900 minutes and the selectivity to light olefins reaches 89%, and the mesopore surface increases. when the amount of ZSM-5 seed or SAPO-18 seed in SAPO-34 precursor were 1% or 5% respectively, the catalysts showed 90 and 85% selectivity to light olefins and a lifetime of 400 and 440 minutes, respectively.

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Electrocatalytical activity of $[(PW_9O_{34})_2Fe_4(H_2O)_2]^{6-}$ polyoxometalate in reduction of NO_2^- ions

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Keywords: Polyoxometalate, Electrochemistry, Electrocatalyst, Reduction, NO_2^-

Polyoxometalates (POMs) are a unique group of molecular metal oxides with distinct physical and chemical properties [1]. Electrochemical researches on polyoxometalate complexes have commonly revealed the presence of an extensive series of reduction processes [2]. The use of POMs in reducing nitrite, iodate, hydrogen peroxide, and bromate has been the subject of numerous investigations during the past decades [3]. This research examines the characteristics of the sandwich-type polyoxometalate $[(PW_9O_{34})_2Fe_4(H_2O)_2]^{6-}$ and evaluates the electrochemistry and electrocatalytic activity of this compound in buffer solutions for the reduction of nitrite ions.

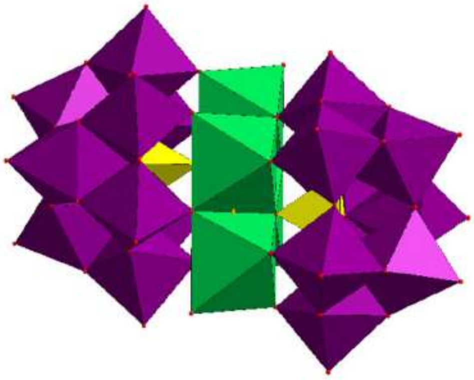

Figure 1: The molecular structure of $[(PW_9O_{34})_2Fe_4(H_2O)_2]^{6-}$.

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A Zn-based coordination polymer with good ability for selective detection of mercury ions in solution

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Keywords: Mercury detection; Sulfur coordination polymer; Zn complex; Methimazole based ligands

$[Zn(NCS)Cl(L)]_n$ (Zn-SCP) is a one-dimensional coordination polymer with a terminal thiocyanate group. The flexible sulfur donor ligand is bridged between metal centers by the anti-anti-anti conformation which forms an infinite 1D zigzag chain and the third and fourth coordination spheres are occupied by terminal Cl^- and NCS^- anions [1]. Considering the HSAB concept (Hard-Soft Acid Base)[2], N-coordinated thiocyanate as a Lewis base has a good potential for coordinating mercury from its free sulfur atom. In this work, we have used Zn-SCP for the detection of Hg^{2+} from water solution with different consecrations. Mercury has been coordinated to the free sulfur of thiocyanate groups as it was excepted. The IR spectrum of Zn-SCP showed a remarkable shift for the NCS peak from 2070 cm^{-1} to 2120 cm^{-1} which clearly shows the change in the coordination sphere. The white color of Zn-SCP powder was changed to grey by coordination with mercury[3]. It is worth mentioning that Zn-SCP has selectivity in the detection of mercury and there were no changes for other metals such as Pb^{2+}, Cd^{2+}, or copper. FT-IR, UV-visible, and ICP have confirmed the binding of mercury to thiocyanate. The Hg^{2+} ions which are coordinated to the Zn-SCP could be removed from the water solution by simple filtration.

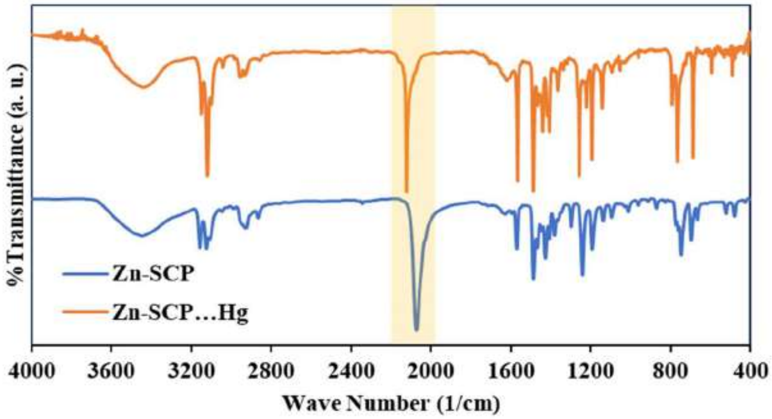

Figure 1. The FT-IR spectra of as-synthesized Zn-SCP and exposed to Hg^{2+} cations.

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Introduction of nickel manganese ferrite nanostructures as highly active nano-photocatalysts for polluted waste water treatment

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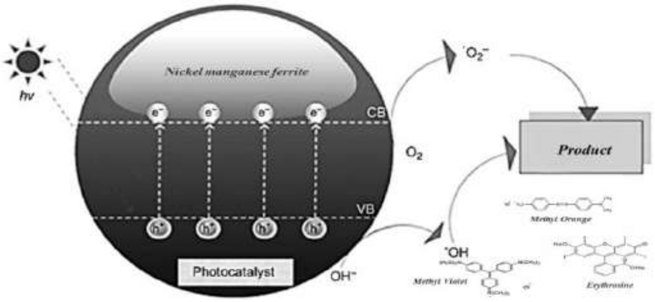
Keywords: Spinel ferrite, Nanostructures, Auto-combustion synthesis, Photodegradation, Organic pollutants

In the present study, we report the auto-combustion synthesis of nanosized nickel manganese ferrite structures through employing a capping agent ligand. The role of ligand as structure-directing agent on the crystal composition and morphological behaviours of as-synthesized spinel ferrites was evaluated. Furthermore, the photocatalytic degradation activity of Ni-Mn ferrite nanostructures as stable semiconductor nano-photocatalysts was explored by decomposing cationic and anionic dyes under simulated light [1-3]. Degrading methyl orange, methyl violet and erythrosine under visible radiation showed discoloration capabilities of 52.35%, 87.03% and 91.62% within 120 min, respectively (**Scheme1**).



Scheme1: Schematic plan of photodegradation efficiency for auto-combustion synthesized Ni-Mn ferrite nanostructures.

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An Organoplatinum(II) Complex Containing Polycyclic Aromatic Hydrocarbon Ligand: Synthesis and Characterization

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Keywords: Platinum, Polycyclic aromatic hydrocarbons, Pyrene derivatives

Polycyclic aromatic hydrocarbons (PAHs) such as pyrene derivatives are good candidates to be used as ligands for the transition metals [1], because they show very different and unusual properties compared to small compounds such as 2-phenylpyridine (ppy) as a result of their extended π-conjugation [2]. Most studies of the incorporation of pyrene derivatives into metal complexes have focused on derivatives substituted at the 1-position, *e.g.*, 1-diphenylphosphinopyrene, due to the ease of their synthesis [3]. Pyrene derivatives functionalized at the 2-position, 2-(2'-pyridyl)pyrene (2-pypyr, **A**), are less well investigated because this position lies on a nodal plane of both frontier orbitals of pyrene and is much more laborious to prepare [4]. This contribution shows the use of the 2-pypyr, **A**, ligand can result in profound differences in the electronic and structural properties of the resultant organoplatinum(II) complex $[Pt(p\text{-}MeC_6H_4)_2(2\text{-pypyr})_2]$, **2**, (**Figure 1**) of the form the Pt(II) complex $[Pt(p\text{-}MeC_6H_4)_2(SMe_2)_2]$, **1**.

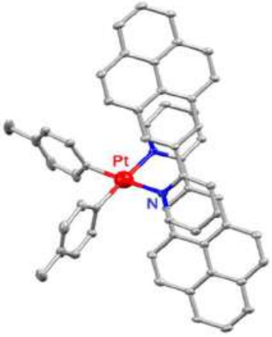

Figure 1. Molecular structure of **2**.

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Combination of bio-based metals and graphitic carbon nitride for pollutant degradation

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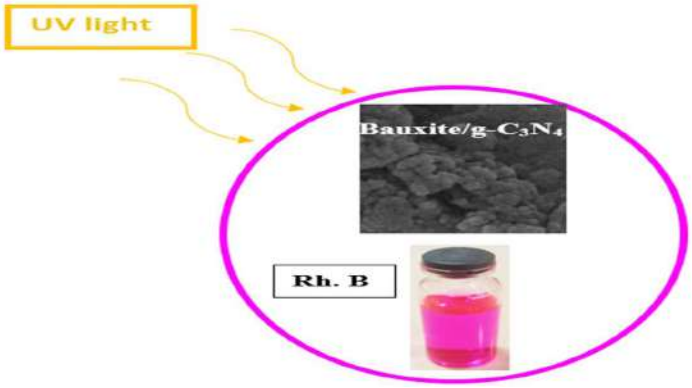
Keywords: Bauxite, g-C_3N_4, Rhodamine B

Environmental challenges are a significant concern in modern society, driving scientists to develop new methods and strategies for designing innovative materials. Graphitic carbon nitride (g-C_3N_4) has emerged as an exceptional polymer with a wide range of applications, including sensors, photocatalysts, and adsorbents, due to its unique properties such as visible-light activity, stability, low cost, and ease of preparation. However, its limitation lies in the low separation efficiency of photogenerated charge carriers, which can be improved by incorporating semiconductor metals. Bauxite is a naturally occurring and heterogeneous material, primarily composed of one or more aluminum hydroxide minerals, along with silica, iron oxide, titania, aluminosilicate, and other minor or trace impurities. Red mud (RM) is a solid waste byproduct generated during alumina production from bauxite [1,2]. In this study, a novel photocatalyst was synthesized using bauxite as a natural source of metals combined with g-C_3N_4 through a simple preparation method, and it was applied for the removal of Rhodamine B (Scheme 1). The resulting composite was characterized using various techniques, and the optimal conditions were determined. The results indicate that the bauxite/g-C_3N_4 composite is highly effective for water purification, achieving a high degradation yield of pollutants.



Scheme1: Removal of Rhodamine B by Bauxite/g-C_3N_4.

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Identification of Optimal Zeolites for Ethyl Mercaptan Removal from Natural Gas by Molecular Simulation

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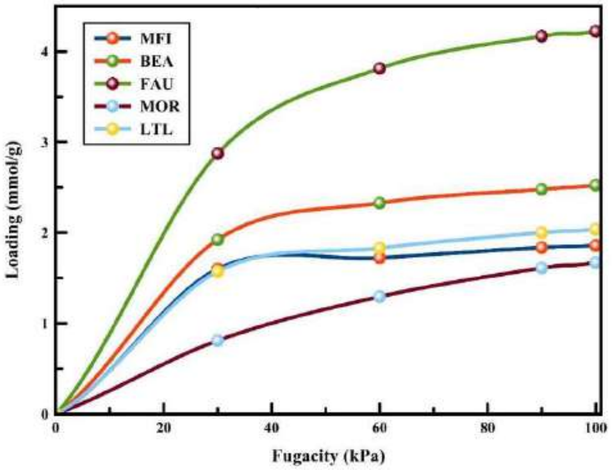
Keywords: Zeolite, Mercaptane, Adsorption, Monte Carlo

The development of suitable compounds for ethyl mercaptan removal from natural gas is one of the main challenges faced by the gas industry. Adsorption on zeolites is a plausible technique to remove mercaptans from natural gas [1]. The adsorption capacities of ethyl mercaptan in the siliceous zeolite frameworks with different topologies were compared. Grand canonical Monte Carlo simulation was employed to gain insight into adsorption mechanisms of ethyl mercaptan in pure and binary mixtures, based on industrial concentration, from adsorption isotherm and distribution of adsorption sites. Adsorption isotherms in the temperature of 298K and pressure ranges of 0-100 kPa, have been simulated. Considering the adsorption capacity, and selectivity of ethyl mercaptan/methane, FAU zeolite has the strongest affinity for ethyl mercaptan adsorption and can thus be efficiently used for deep desulfurization of natural gas.



Scheme1: The simulated adsorption isotherm of ethyl mercaptan in the binary mixtures of mercaptans and methane on BEA, FAU, LTL, MFI, and MOR zeolites.

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Activated carbon synthesized from olive stones for removal of methylene blue dye from wastewater

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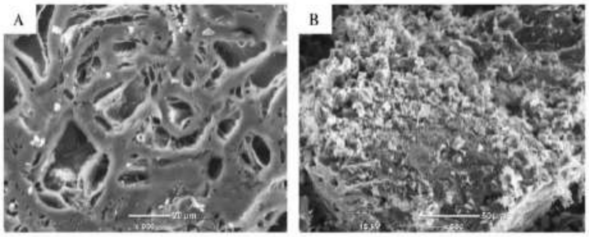
Keywords: Activated carbon, Wastewater treatment Adsorption, Textile dye

Growing urbanization has led to production of significant amounts of complex wastewater containing resistant inorganic and organic pollutants. As conventional treatment methods fail to effectively minimize the concentrations of resistant pollutants to meet desired levels, the demand for innovative tertiary treatment solutions continues to grow. Adsorption has emerged as a favored tertiary treatment technique due to its high removal performance, diverse applications and ease of use. Activated carbon is particularly popular because of its large specific surface area. High stability and easy synthesis routes [1]. Scanning electron microscopy revealed that the activated carbon had deep cavities that were filled after the adsorption of methylene blue. Fourier transform infrared spectroscopy showed various functional groups present on the activated carbon before and after the adsorption process. **CHN analysis,** indicated that the highest percentages of nitrogen, hydrogen, and carbon were found in black olive stone activated carbon. Additionally, the results showed that the optimal pH value for methylene blue adsorption was 10, where the dye was adsorbed at its highest rate [2].



Scheme1: SEM image of black ACOS (A) before MB adsorption and (B) after MB adsorption at different scale 20 and 50 µm.

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Polypyridyl materials as a versatile platform for light-emitting electrochemical cell

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Keywords: Polypyridyl ligands, Phenanthroimidazole, Light-emitting electrochemical cell

Light-emitting electrochemical cells (LECs) are thin film lighting devices that consist of one or two ionic-based active layers sandwiched between two air-stable metal electrodes. These devices exhibit some interesting features that may make them more favourable compared with traditional organic light-emitting diodes (OLEDs), which allow the non-rigorous encapsulation of devices [1]. Among all-luminescent materials, ionic transition metal complexes (iTMCs) have received more attention due to their promising advantages such as their stable redox properties, and highly efficient phosphorescence nature of emission [1]. However, LEC devices suffer from low stability and long response time, limiting their practical applications. Chemical modification of iTMCs has been used to overcome these limitations. In our works, the phenanthroline with a fused imidazole unit with high chemical modification potential was employed as ligand and molecularly-engineered switches (**Figure 1**) [1-3].

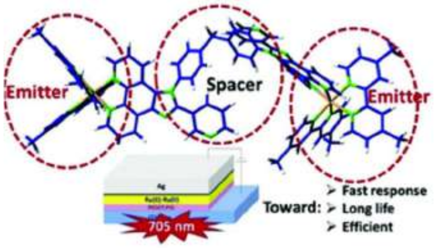

Figure 1: Near-infrared binuclear ruthenium (II) PI-based complex and LEC device [3].

In this context, a combinational approach such as electron donor/acceptor substitutions, various ancillary ligands, binuclearization strategy, and tethered ionic group is used for optimization of efficiency, stability, and response time of both ruthenium (II) and cyclometalated iridium (III) complexes-based LEC devices [1-3]. Our research confirms the advantages of employing these polypyridyl materials to modify iTMC emitters for LECs.

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Inhibiting the interaction of SARS-COV-2 virus S protein and human ACE2 protein with a molecular docking approach

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Keywords: ACE2, S Protein, RDB, SARS-CoV-2, Molecular Docking.

Human Angiotensin-Converting Enzyme 2 (ACE2) is the primary receptor for the SARS-CoV-2 virus, which enters the lower respiratory tract's epithelial cells. It interacts with the Receptor-Binding Domain (RBD) of the SARS-CoV-2 protein S [1,2]. In this study, we used a computational method to investigate whether natural small molecules derived from the ginger plant can inhibit the interaction between the RBD domain of the SARS-CoV-2 virus S protein and the human ACE2 protein. We employed Autodock (1.5.6) software to perform molecular docking between the three-dimensional structure of the RBD domain protein of the virus (receptor) and 41 active compounds from ginger (ligand). Molecular docking allows us to predict the interaction between the receptor protein and biologically active compounds and identify factors that contribute to a stable and significant interaction for drug recognition. Additionally, we calculated the binding affinity (Kcal/mol) of the 41 ginger compounds to the RBD of the SARS-CoV-2 protein. One of these compounds, citral, exhibited a binding affinity of -3.9 Kcal/mol (Figure 1). These compounds have the potential to effectively prevent virus entry, replication, and multiplication within cells. Therefore, they represent promising candidates for further in vitro and in vivo studies.

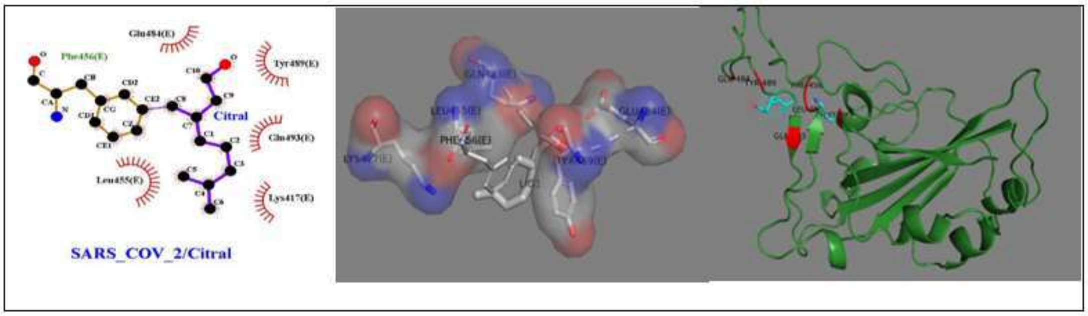

Figure 1: Interaction of protein s from SARS-Cov2 virus and ACE2 protein from humans with citral compound from ginger.

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Computational modeling to investigate the photovoltaic performance of a new class of perovskite $(C_6H10N_2)[CuCl_4]$ 2D-type

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Keywords: Perovskite, Computational modeling, DFT, TD-SCF, Photovoltaic/solar cell

Today, photovoltaic and solar cells are widely used in microelectronic and nanotechnology [1,2]. In this study, the electronic/vibrational structure and some optoelectronic properties of a sample 2D type complex $(C_6H_{10}N_2)$ $[CuCl_4]$, **Figure 1**, are calculated, in order to evaluate it for use in solar cell systems, using density functional theory (DFT) at B3LYP/6-311G(d,p) level of theory. In this regard, the molecular vibration frequency, the (E_{HOMO}-E_{LUMO}) molecular energy gap, molecular density of states (DOS), power conversion efficiency (PCE) and fill factor (FE) of this 2D-type nano-size complex were calculated, using G09 software. In addition, some optoelectronic properties of this complex such as λ_{max}, excitation energy (Ex), excitation energies and light-harvesting efficiency (LHE) were calculated, based on the time-dependent self-consistent field method (TD-SCF). The analysis of the obtained results, such as reported in **Table 1.,** showed that this complex can be a suitable option for use in solar cell systems.

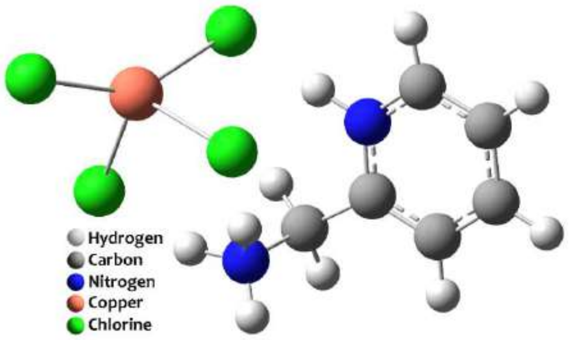

Fig. 1. Optimized structures of complex $(C_6H_{10}N_2)[CuCl_4]$ 2D-type perovskite

Table 1. Theoretically calculated values for open circuit voltage (V_{oc}), normalized V_{oc}, fill factor (FF), and power conversion efficiency (PCE) for $[C_6H_{10}N_2]CuCl_4$ complex.

Voc (eV)	Normalized V_{oc}	FF	PCE%
2.6	100.37	88.26	25.81

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Synthesis and Evaluation of Anticancer Activity of a Novel Cyclometalated Platinum(II) Complex with Enhanced Selectivity

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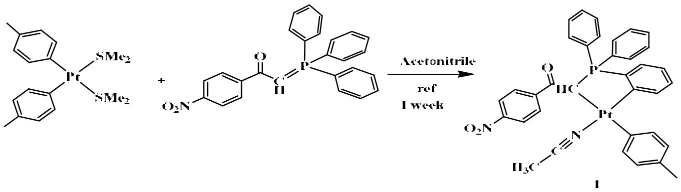
Keywords: Cyclometalated, Platinum, Phosphonium Ylide.

Cancer remains one of the leading causes of death globally, driving extensive research into new treatment methods and anticancer drugs. Among these treatments, platinum-based chemotherapy drugs are particularly significant, motivating the search for complexes that offer comparable cytotoxicity with fewer side effects [1]. This study focuses (**Scheme1**) on the synthesis and characterization of a cyclometalated Pt(II) complex, [Pt(*p*-MeC_6H_4)(YPN)(CH_3CN)], **1**, which is derived from [Pt(*p*-$MeC_6H_4)_2(SMe_2)_2$] [2] and a phosphonium ylide ligand, YPN, $Ph_3PC(H)C(O)C_6H_4NO_2$ [3]. The cytotoxicity of **1** was assessed across various human cancer cell lines, including A549 (lung), MCF-7 (breast), and HeLa (cervical), as well as a normal lung fibroblast cell line (MRC-5) [4]. The results revealed promising anticancer activity, with a selective effect on cancer cells, particularly in MCF-7 cells. Notably, complex **1** showed greater selectivity for cancerous cells compared to cisplatin and also induced apoptosis, highlighting its potential as an effective anticancer agent.



Scheme 1. Synthetic routes for the preparation of **1**.

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Facile fabrication, characterization, and photocatalytic performance of zinc manganese ferrite nanostructures under simulated light

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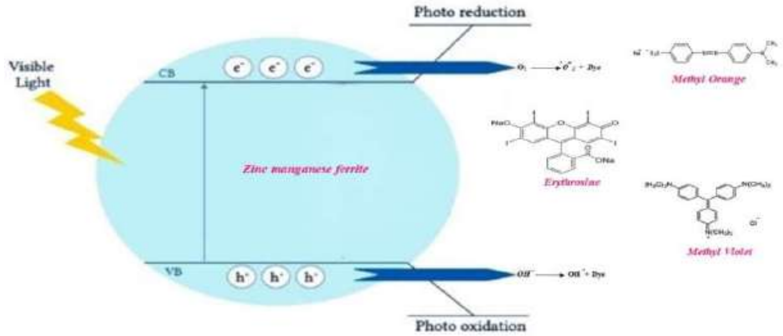
Keywords: Zn-Mn ferrite, Spinel nanostructure, Auto-combustion synthesis, Toxic pollutant, Photocatalytic activity

To fabricate a mixedmetallic oxide based on spinel Zn-Mn ferrite nanostructures, an efficient sol–gel auto-combustion route was utilized under alkaline media. The influence of Schiff-base ligand on the crystal structural, morphological and particle size distribution of the nano- Zn-Mn ferrite was investigated in detail. Since the organic contamination in the water are known as serious problem in the society [1, 2], we aim to investigate the activity of Zn-Mn ferrite nanostructures as photocatalytic substances through elimination of three different types of dyes such as: erythrosine, methyl orange, and methyl violet under visible light (**Scheme1**). After 120 min, the maximum decolorization efficiency was obtained as 96.96% for erythrosine.



Scheme1: Rational design and photocatalytic activity for auto-combustion synthesized Zn-Mn ferrite nanostructures by employing Schiff-base ligand.

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New polymeric electrodes for non-enzymatic detection of glucose

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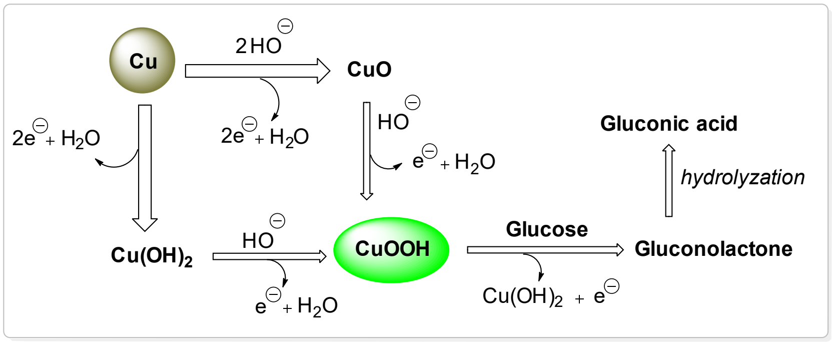
Keywords: Non-enzymatic Sensor, Polymeric Electrode, green chemistry, Electrochemical Oxidation, Glucose Oxidation

Flexible non-enzymatic glucose sensors made of textiles monitor glucose levels in sweat, tears, and blood, which are useful for health diagnostics.[1] High blood glucose levels are one of the most important and serious global threats to human health [2]. Therefore, it is highly desirable to develop new technologies to solve this problem [3]. In this study, it was decided to design, fabricate, and characterize a highly stable polymer electrode with suitable conductivity and porosity for glucose detection. To achieve this, fibrin protein deposited on pure cotton fabric was used as a biological polymer substrate. Electrode conductivity was optimized for electrochemical processes through several steps, including rGO additives, linkers, and copper metal incorporation into the polymer substrate. The results showed that the introduced electrode has high stability and strength, high porosity, wedge-shaped voids, and sufficient conductivity.



Scheme 1: Proposed mechanism of the detection of Glucose onto the introduced electrode.

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Fabrication of new composite electrode for electrosynthesis of hydrogen peroxide

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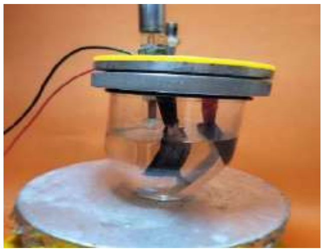
Keywords: Polymeric Electrode, green chemistry, Electrochemical Oxidation, Hydrogen peroxide

The synthesis of hydrogen peroxide (H_2O_2) is a vital chemical process with significant applications in various industries, particularly in medicine, where it acts as a powerful oxidizing agent for purification and disinfection. H_2O_2's unique properties make it valuable in the pharmaceutical industry and in the production of other chemicals, thereby enhancing health outcomes and process efficiencies [1]. Recent advancements in the design of polymeric composite electrodes, leveraging natural polymers like chitosan and silk fibroin, have emerged as promising solutions due to their non-toxicity, environmental compatibility, and strength. In a recent study, a composite electrode was developed using fibrin protein, graphene oxide, and Cu which exhibited excellent conductivity and porosity [2]. This electrode was tested for its efficiency in the electrochemical synthesis of H_2O_2, achieving high concentrations of approximately 0.3 M in a 0.6 M sulfuric acid environment. The results highlight the potential of these composite materials to enhance H_2O_2 production, contributing to innovative applications in industrial and healthcare contexts(**Scheme1**).



Scheme 1: An overview of the electrochemical cell for the synthesis of hydrogen peroxide.

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A novel complex of Co(II) with pyrazine-2-carboxamide derivative ligand; synthesis, characterization & single crystal X-ray diffraction studies

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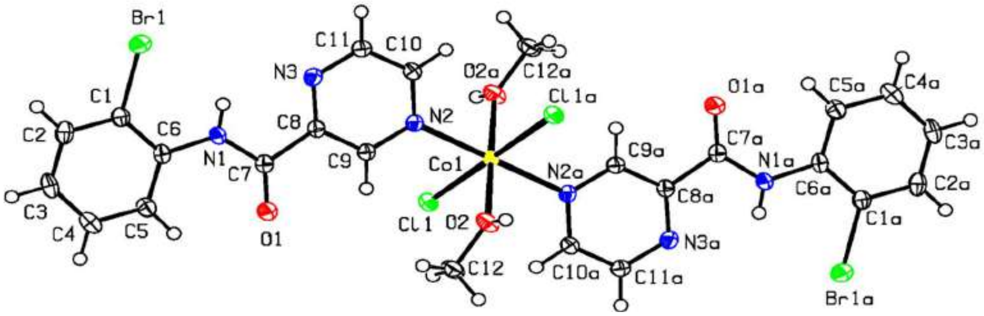
Keywords: Synthesis, Carboxamide, Single-crystal, Co(II)

In chemistry and biology, the peptide group –C(O)NH– is an important forming unit. In 2023, synthesis and characterization of a new Co(II)–carboxamide complex has been reported [1,2]. In this study, a new Co(II) complex, $[Co(L^{2Br})_2(Cl)_2(CH_3OH)_2]$ (**1**) (where L^{2Br} is *N*-(2-bromophenyl)pyrazine-2-carboxamide) have been synthesized. The complex characterized by single crystal X-ray diffraction method and IR spectroscopy. In addition, the L^{2Br} was characterized by ^{1}HNMR spectroscopy. According to the crystal data, this complex crystallizes in triclinic space group $P\overline{1}$ and unit cell volume of 671.52(19) Å^3. Each central Co(II) has an octahedral geometry formed by two N-donor atoms of two pyrazine rings, two chloride anions and two oxygen atoms of methanol. (**Scheme1**).



Scheme1: ORTEP drawing (50% probability displacement ellipsoids) of complex **1** with the atom numbering scheme. Symmetry code: (a) 1-x,2-y,-z.

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Preparation of lithium manganese iron phosphate compounds for use in lithium-ion batteries

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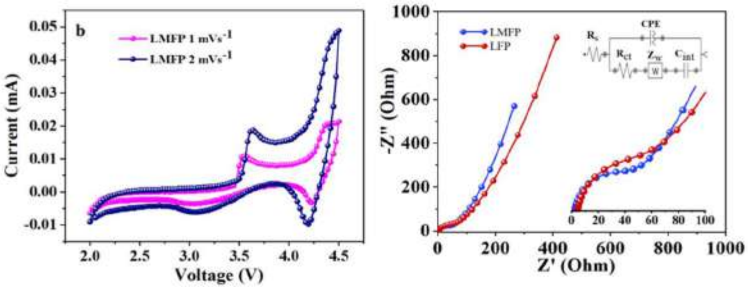
Keywords: Lithium manganese iron phosphate, Cathode, Lithium-ion battery, Electrochemical performance, Cyclic voltammetry.

Today, rechargeable lithium batteries are widely used as a power source for portable electrical devices, phones and mobile computers. A wide range of lithium iron phosphate oxides have been considered for use in these batteries as cathodes. LFP(Lithium iron phosphate) has obvious advantages such as: low cost, high security, good stability, environmental friendliness and energy saving, as a result it has been widely used in the manufacture of electric vehicle batteries. However, it still has disadvantages such as low lithium-ion transfer rate (1011 cm2/s) and low conductivity (109 siemens). These disadvantages limit its charge and discharge efficiency to a high extent [1]. In this research work, cathode material LFPO4(Lithium iron phosphate) and LMFPO4(Lithium manganese iron phosphate) were synthesized by chemical hydrothermal method. The synthesis of the samples was confirmed by X-ray diffraction analysis (XRD) and Fourier-transform infrared spectroscopy (FT-IR) analyses. The performance of these cathode materials in the battery was investigated using cyclic voltammetry (CV) and electrochemical impedance spectroscopy [2].

For this purpose, cyclic voltammetry test of LFP, $LM_{0.7}F_{0.3}P$, $LM_{0.75}F_{0.25}P$, $LM_{0.5}F_{0.5}P$ and $LM_{0.8}F_{0.2}P$ samples was performed in 1 M $LiNO_3$ aqueous electrolyte. LFP and LM0.7F0.3P samples had a current of 40.34 and 71.76 mA h, which have a capacity of about 134.47 and 199.33 $mAhg^{-1}$. In the final stage, LFP and $LM_{0.7}F_{0.3}P$ samples, which had better capacity, were placed in the organic electrolyte system by cyclic voltammetry and electrochemical impedance testing; The capacity of LFP and $LM_{0.7}F_{0.3}P$ were obtained as 41.95 and 104.81 $mAhg^{-1}$, respectively. The reason for this behavior is the correct percentage ratio of manganese and iron in the synthesis of lithium manganese iron phosphate **(Scheme1)**.



Scheme1: (a) Cyclic voltammetry plots of $LM_{0.7}F_{0.3}P$ at scan rates of 1 and 2 mV/s, (b) Nyquist curve of LFP and $LM_{0.7}F_{0.3}P$ electrodes.

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Highly efficient electrochemical sensing acetaminophen based on metal organic framework

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Keywords: Acetaminophen, Electrochemical sensor, Cyclic voltammetry

Acetaminophen, with the chemical name N-acetyl-p-aminophenol (AP), is a widely used analgesic and antipyretic. It is considered safe when administered in recommended doses. However, it can cause hepatotoxicity and side effects in higher doses [1]. For this reason, the development of a simple, fast, sensitive, and accurate analytical technique for the determination of AP in drugs and clinical preparations is necessary. Various methods such as titrimetry, spectrophotometry, and HPLC have been developed for the determination of AP in pharmaceutical tablets and biological fluids. However, titrimetric and spectrophotometric methods involve tedious extraction processes before detection. In addition, liquid chromatography is time-consuming, which makes it unsuitable for the analysis of AP in practice. On the other hand, electrochemistry offers powerful analytical techniques with advantages such as instrument simplicity, moderate cost, and portability [2]. MOFs as suitable candidates show very good performance in electrochemical activities, so that in this research, Zn-MOF, which has zinc metal nodes, is used to detect AP [3]. In this way, once the unmodified glassy carbon electrode (GCE) and the modified electrode with Zn-MOF were checked in 0.1 M phosphate buffer, pH = 7 in the absence of the drug and the second time in the presence of the drug by cyclic voltammetry. The results showed that no peak was observed in the absence of the drug, but in the presence of the drug, a current of 12.2 μA and a peak at 0.58 V were reported for GCE, and a higher current of 21 μA and a peak at 0.52 V were reported for Zn-MOF/GCE, which indicates the good electrocatalytic activity of the proposed electrode in the determination of acetaminophen as a drug sensor.

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Synthesis, characterization and study of physical and optical properties of diatomite modified with indium oxide

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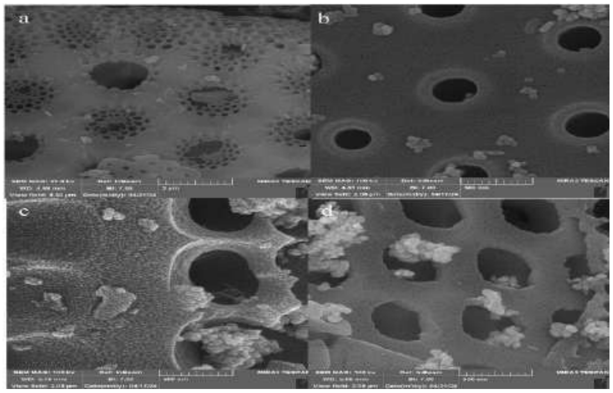
Keywords: Diatomite, Color removal, Indium oxide, Sonochemical method, Photocatalyst

In_2O_3-modified diatomite nanomaterials with different indium oxide contents were prepared via an efficient sonochemical technique. The as-prepared compounds products were analyzed by means of energy dispersive X-ray photoelectron spectroscopy (EDX), scanning electron microscopy (SEM), X-ray diffraction (XRD) and Brunauer-Emmett-Teller (BET) techniques. As indicated by XRD, diatomite phase and indium oxide peaks were observed. The BET specific surface area and pore volume of In_2O_3-coated diatomite is greater than pure diatom. The surface morphology and high porosity of diatom can be utilized as the template to boost potential of functional materials. The photocatalytic activities of as-prepared compounds were assessed for the decolorization of methylene blue. The results revealed that diatomite modified with indium oxide can be used in different experimental runs with no essential drop in photocatalytic activity.



Scheme1: SEM images of natural diatomite (a), diatomite modified with indium oxide at different stoichiometric ratio (b-d).

References

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Synthesis and investigation of photocatalytic properties of manganese oxide nanoparticles doped with lanthanide cation

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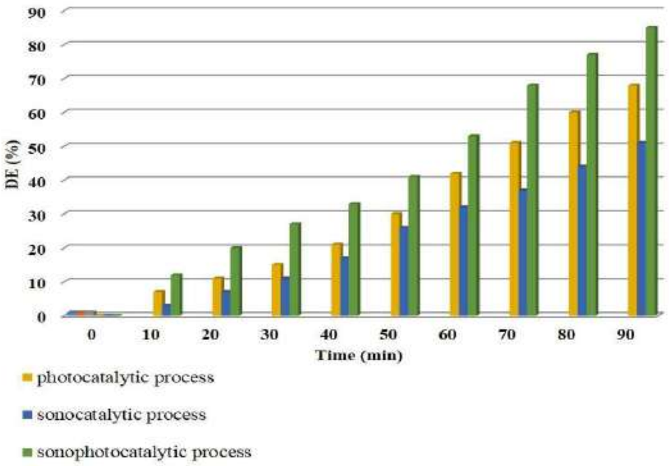
Keywords: Hydrothermal, Manganese oxide, Photocatalyst, Semiconductor.

In this study, nano-structured manganese oxide compounds doped with gadolinium cations were prepared by effective hydrothermal method. XRD, SEM and DRS absorption spectroscopy techniques were used to identify the synthesized materials. According to the X-ray diffraction patterns, the prepared materials have a spinel manganese oxide crystal structure. The photocatalytic properties of the prepared samples were used and evaluated to remove the methylene blue dye under the photocatalytic and sonophotocatalytic process in aqueous medium. Experiments show that with the increase in the amount of dopant, the percentage of color removal has increased and the highest value obtained for pollutant removal is related to the sample of manganese oxide doped with gadolinium (x=0.08). Also, the role of several factors such as color concentration, catalyst amount and photocatalytic process time were studied.



Scheme1: Comparison of different processes in the removal of methylene blue dye considering the following conditions: [Dye] = 20 mg/L, [Catalyst] = 1 g/L.

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Two Schiff-base complexes of zirconium oxide and copper fabricated on magnetic nanoparticles as efficient and reusable catalysts in the synthesis of amide derivatives

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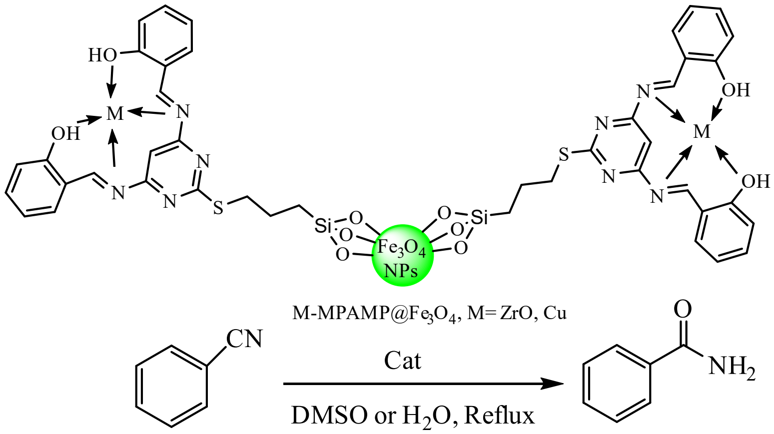
Keywords: Fe_3O_4 magnetic nanoparticles; Schiff-base complex; heterogeneous catalysts, zirconium oxide; copper; amide

Two Schiff-base complexes of zirconium oxide and copper on Fe_3O_4 magnetic nanoparticles were synthesized. Then, their catalytic performance were developed in the synthesis of amide derivatives by reduction of nitrile to amide. These catalysts were characterized using SEM, WDX, EDS, TGA, XRD, AAS and VSM techniques. The characterized analysis confirmed that these heterogeneous catalysts are stable during the reaction process and could also be reused several times. The amide products were obtained in good to excellent yields with high purity (**Scheme 1**).



Scheme 1: Synthesis of amides in the presence of M-MPAMP@Fe_3O_4 (M=ZrO or Cu).

References

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Synthesis of two-dimensional polymers based on hPG and investigation of its theoretical calculations

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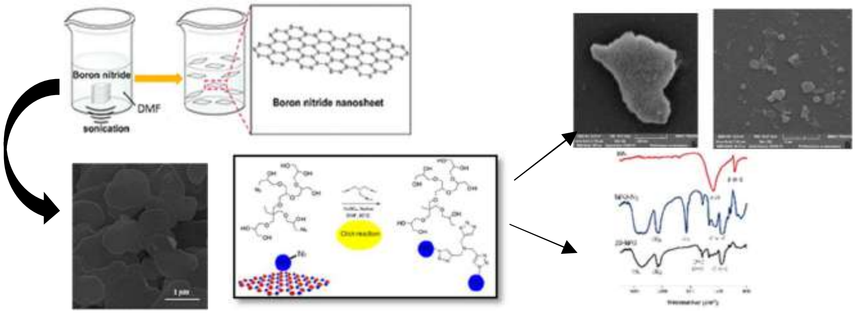
Keywords:TWO- Dimensional polymer, polyglycerol, FT-IR, FESEM, Theoretical Calculattions.

Synthetic 2D nanomaterials (2DNs) have attracted wide attention in the past several years, due to the possibility of tuning their physicochemical and optoelectronic properties by manipulating their structure and functionality [1] In this work, boronnitrid sheets were used as flexible templates to construct 2D polyglycerols in solution. In this synthetic strategy, polyglycerol branches with 10% azide groups (hPGN3(10%)) were conjugated to the surface of boron nitrid sheets by pH sensitive linkers and they were laterally crosslinked by a copper-catalyzed click reaction. Tripropargylamine was adsorbed on the surface of polyglycerol functionalized boronnitrid sheets and used as acrosslinker.The association of tripropargylamine with the boron nitrid surface and lifting off this reagent by a controlled heating diminished the risk of intersheet crosslinking and resulted in 2D polyglycerol upon acidification and centrifugation. After synthesizing the polymer, its structure was confirmed employing the IR spectrometry and then its morphology was studied using the FESEM methods. A theoretical calculation was used to investigate interaction between the polyglycerol and the BN nanosheet. As consequence, it was found that the weak exothermic ineraction exist between the polymer and BN Nano sheet (**Scheme1**)



Scheme1: Graphical Synthesis of two-dimensional polymers based on hPG.

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Copper complex of 1-(benzo[d]thiazol-2-yl)urea immobilized on mesoporous SBA-15 as an efficient catalyst for preparation of 5-substituted 1H-tetrazoles

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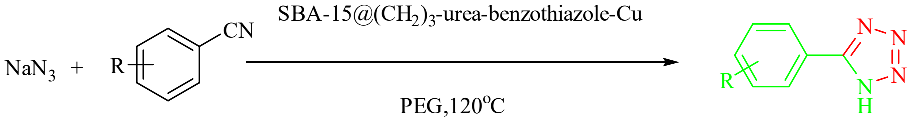
Keywords: Mesoporous SBA-15; 1-(benzo[d]thiazol-2-yl)urea; heterogeneous catalysts, tetrazoles; copper.

In this study, a green and efficient catalyst was prepared by immobilization of copper complex of 1-(benzo[d]thiazol-2-yl)urea on the surface of mesoporous SBA-15 (SBA-15@(CH$_2$)$_3$-urea-benzothiazole-Cu). At frist, 1-(benzo[d]thiazol-2-yl)urea as a new ligand was immobilized on the surface of modified SBA-15, and further it was used as an effective host for the immobilizing Cu(II) ions. The synthesized catalyst was characterized by XRD, SEM, WDX, BET, EDS, and FT-IR, and then successfully used to synthesize 5-substituted tetrazoles. In synthesizing 5-substituted 1H-tetrazoles, the catalyst shows high yields in short reaction times at 120 °C (Scheme 1). Also, the prepared catalyst showed high reusability, which it was reused 5 times without significantly decreasing in its catalytic activity.



Scheme 1: Synthesis of 5-substituted tetrazoles in the presence of SBA-15@(CH2)3-urea-benzothiazole-Cu.

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Green synthesis of Fe and Zn metal-organic frameworks and their application in electrochemical supercapacitors

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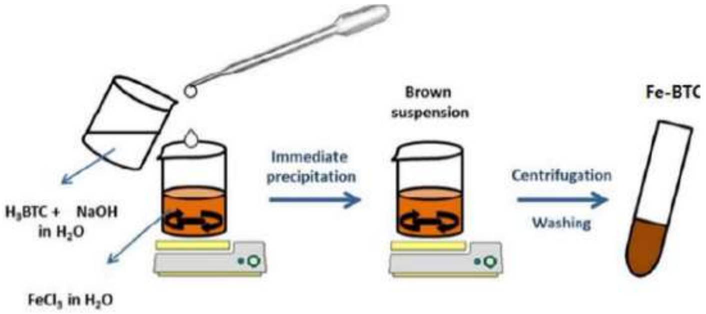
Keywords: Metal-Organic-Frameworks, Supercapacitors, Green synthesis, Electrochemistry

Supercapacitors have attracted significant attention due to their high power density and rapid charge/discharge capabilities, which are critical for energy storage applications. In this study, iron and zinc-based metal-organic frameworks (MOFs) with 1,3,5-benzene tricarboxylic acid ligands were synthesized using a green method at ambient and hydrothermal conditions to design high-capacity supercapacitors. Environmentally friendly solvents, water and ethanol, were employed to reduce environmental impact. The materials were characterized using FT-IR, XRD, and SEM. Composite electrodes were prepared by mixing the MOFs with graphite and paraffin and tested in a three-electrode system. The POAP/Fe-BTC and POAP/Zn-BTC composites demonstrated superior specific capacity and energy efficiency compared to traditional electrodes. The POAP/Fe-BTC Hydrothermal electrode showed the best performance.



Scheme 1: Schematic illustration of the synthesis process for Fe-BTC at room temperature.

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Synthesis and characterization of ZIF-9@CoAl LDH nanocomposite and investigation of its catalytic properties for the degradation of methylene blue dye via the activation of Potassium peroxymonosulfate salt

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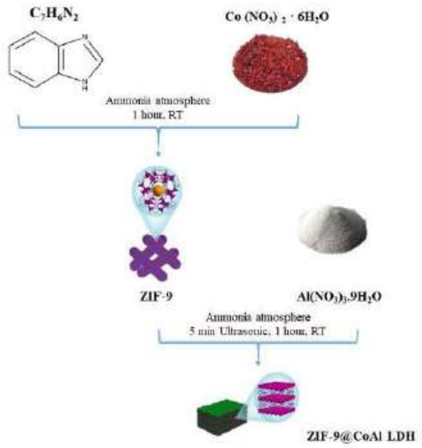
Keywords: Nanozeolitic imidazolate frameworks, Layered double hydroxides, Catalyst

Zeolitic imidazolate frameworks (ZIFs) are an emerging subset of metal-organic frameworks (MOFs) known for their high porosity and specific surface area. Applications of ZIFs include sensors, drug delivery and catalysis. In this study, ZIF-9 was synthesized, and by incorporating a second trivalent cation, layered double hydroxides(LDH) were formed, resulting in the synthesis of ZIF-9@LDH nanocomposites. Characterization of the products was performed using FT-IR, XRD, FE-SEM, EDX, and BET techniques .These nanocomposites exhibited a significantly higher specific surface area and were used for the degradation of methylene blue dye. The ZIF-9@LDH/PMS system achieved 97% dye degradation via the main radical species ($SO_4^{\bullet -}$ and $^1O_2$), as confirmed by UV-visible spectroscopy, demonstrating its potential for environmental remediation.



Scheme1: Schematic illustration of the synthesis process for ZIF-9 and ZIF-9@CoAl LDHs

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Absorption Removal of Gabapentin by modified Zr-based MOF “UIO-66” from water and wastewater treatment

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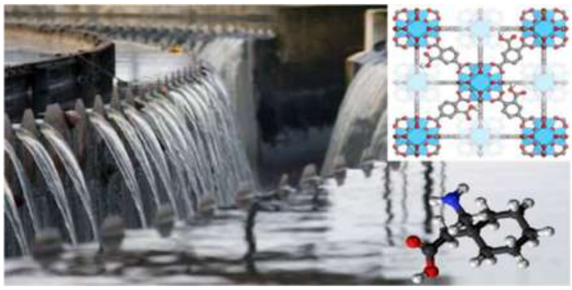
Keywords: Metal-organic frameworks, UIO-66, Water treatment, Nanoparticle

Growing population and social advances makes accessibility limits to drinking water. To achieve this goal, drinking water, applying efficient technologies is important. Nano technology is one of the most important technologies, providing fundamental solutions to make drinking water from waste water containing pollutants such as dyes, heavy metals, pharmaceutical contaminants and etc. One of the most promising techniques for recycling pollutants is adsorption of pollutants by nanoparticles. Gabapentin is a common anticonvulsant drug that poses a potential risk to the environment due to its ability to accumulate in water systems over time and impact aquatic life and ecosystems negatively. Therefore, it is crucial to implement efficient water treatment methods to safeguard the environment and preserve the quality of water sources by removing gabapentin from wastewater effectively. In this study, the ability of modified Zr-based MOF (UiO-66) to remove Gabapentin from aqueous solution was studied [1]. The modified UiO-66 demonstrated removal efficiency more than 90% and high adsorption capacity in comparison to previous samples [2]. The obtained data was investigated and analyzed by infrared spectroscopy (IR), Brunauer-Emmet-Teller (BET), Ultra-violet spectrophotometry (UV-Vis), and X-Ray diffraction (XRD).



Scheme1: Graphical abstract of adsorption removal of gabapentin from wastewater.

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Synthesis, Characterization and Cytotoxicity Evaluation of n-ZnO, ZnO/chitosan and ZnO/Cellulose Nanocomposite via Sol-gel Method on HGF cell line

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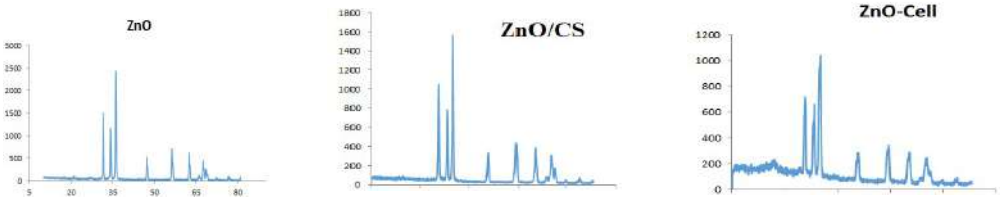
Keywords: MTT, n-ZnO, n-ZnO/chitosan, Nanocomposite, Sol-gel

Nanostructured ZnO (n-ZnO) has gained remarkable attention for excellent properties compared to other metal oxides [1]. Sol-gel method is one of the most effective methods used for nano-rod and nano-sphere ZnO [2]. In this method, uniform, homogenies, and ultrafine nano crystals often is obtained. In light of the above background, the present investigation was aimed to synthesize biocompatible ZnO/chitosan (ZnO/CS) and ZnO/Cellulose (ZnO/Cell) nanocomposite for dental application. In order to determine the in-vitro viability of these synthesized nanocomposite on HGF normal cell, the MTT assay test was used [3]. Figure 1 explain the XRD of these nanostructures was shown **(Scheme1**).



Scheme1: The XRD diffraction pattern of the synthesized ZnO NPs, n-ZnO/CS and n-ZnO/Cell nanocomposite

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Copper sulfide nanostructures and nanocomposites: synthesis, characterization and investigation of the photocatalytic applications

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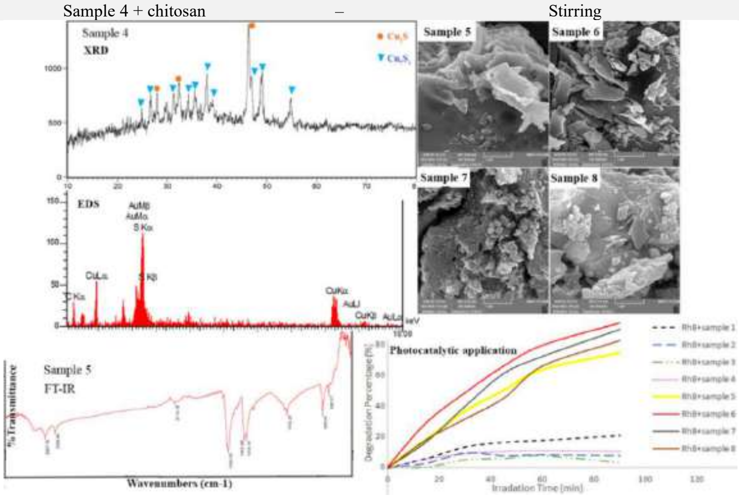
Keywords: Nanocomposite, Copper sulfide, Chitosan, Photocatalyst.

Copper sulfide (Cu_xS_y) nanostructures have garnered significant attention due to their versatile properties and potential applications in various fields such as electronics, energy storage, and catalysis [1]. This interest stems from their unique electrical, optical, and thermal characteristics, which can be finely tuned through the manipulation of their size, shape, and composition. The focus of this research was on preparing Cu_xS_y nanostructures and nanocomposites, and evaluating their potential as photocatalysts for the degradation of organic dyes. Cu_xS_y/chitosan nanocomposites were synthesized after three steps, including reflux, thermal decomposition and stirring. Chitosan was used in this research. Scheme 1 presents XRD, SEM and EDS results of the synthesized products. To evaluate the photocatalytic properties of the samples, experiments were conducted involving the photodegradation of Rhodamine B (RhB) dye under visible light.

Table 1. The reaction conditions of Cu_xS_y nanostructures and Cu_xS_y/chitosan nanocomposites.

Sample	Precursors	Capping agent	Synthesis method	T and t of calcination
1	$Cu(NO_3)_2$ + Tu	–	Thermal decomposition	500 °C , 4h
2	$Cu(NO_3)_2$ + Tu	CTAB	Thermal decomposition	500 °C , 4h
3	$Cu(NO_3)_2$ + Tu	PEG4000	Thermal decomposition	500 °C , 4h
4	$Cu(NO_3)_2$ + Tu	PVA	Thermal decomposition	500 °C , 4h
5	Sample 1 + chitosan	–	Stirring	–
6	Sample 2 + chitosan	–	Stirring	–
7	Sample 3 + chitosan	–	Stirring	–
8	Sample 4 + chitosan	–	Stirring	–



Scheme 1: XRD, SEM, EDS, FT-IR and photocatalytic applications of Cu_xS_y nanostructures and Cu_xS_y/chitosan nanocomposites.

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Synthesis, characterization and investigation of the photocatalytic properties of lead sulfide nanostructures and nanocomposites

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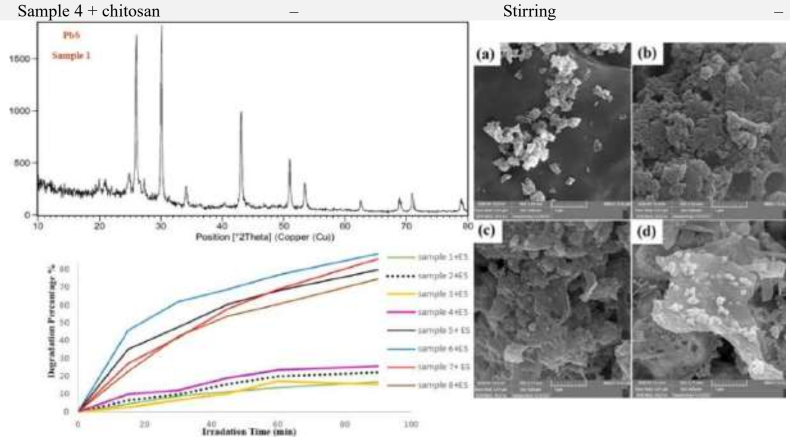
Keywords: Nanocomposite, PbS, Thermal Decomposition, Photocatalyst.

In recent times, the study of chalcogenide semiconductors, particularly on a nano level, has seen a surge in interest within the realm of materials science [1]. This heightened focus can be attributed to the significant transformations observed in the material's electrical, thermal, and optical properties, suggesting substantial potential for widespread technological progress. Lead sulfide (PbS) has applications in the development of advanced photodetectors, sensors, and systems for infrared imaging. In this research, PbS nanostructures and nanocomposites were prepared via thermal decomposition and stirring. Various analytical techniques were used to characterize the materials' structure and composition. Then photocatalytic properties of them are investigated for degradation of erythrosine (ES). The photocatalytic experiments were conducted under visible light. Table 1 shows different conditions for synthesizing the nanostructures and nanocomposites.

Table 1. The reaction conditions of PbS synthesized in this research.

Sample	Precursors	Capping agent	Synthesis method	T and t of calcination
1	$Pb(NO_3)_2$ + Tu	–	Thermal decomposition	500 °C , 4h
2	$Pb(NO_3)_2$ + Tu	CTAB	Thermal decomposition	500 °C , 4h
3	$Pb(NO_3)_2$ + Tu	PEG4000	Thermal decomposition	500 °C , 4h
4	$Pb(NO_3)_2$ + Tu	PVA	Thermal decomposition	500 °C , 4h
5	Sample 1 + chitosan	–	Stirring	–
6	Sample 2 + chitosan	–	Stirring	–
7	Sample 3 + chitosan	–	Stirring	–
8	Sample 4 + chitosan	–	Stirring	–



Scheme 1. XRD, SEM and the photocatalytic properties of PbS nanostructures and nanocomposites prepared under different conditions.

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SnO_2 photocatalyst: synthesis via three methods and investigation of the photocatalytic applications

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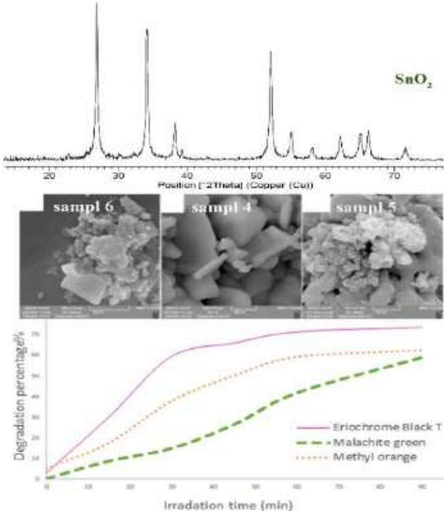
Keywords: SnO_2, Co-precipitation, Hydrothermal, Sol-gel, Photocatalyst.

The metal oxide semiconductors, particularly SnO_2, are crucial in advanced technologies due to their unique properties [1, 2]. SnO_2 includes broad bandgap, exceptional stability, and versatile applications ranging from sensors to energy storage devices. The SnO_2 is an n-type semiconductor with a band gap between 3.6 and 4.0 eV. This study focuses on synthesizing SnO_2 nanostructures via three different methods, including hydrothermal, sol-gel, and co-precipitation. Table 1 shows different conditions for synthesizing the nanostructures. The nanostructures were characterized and used as photocatalyst for the degradation of the organic dyes. Fig. 1 shows XRD patterns and SEM images of the products. In relation to the photocatalytic property of the samples, photodegradation of Malachite green, Methyl orange, and Eriochrome black B dyes was performed under UV irradiation.

Table 1. The reaction conditions of $SnCl_2$ synthesized in this work.

Sample	Precursors	Capping agent	Synthesis method	T and t of Calcination
1	$SnCl_2.2H_2O$	CTAB	Co-precipitation	350 ˚C , 2h
2	$SnCl_2.2H_2O$	PEG4000	Co-precipitation	350 ˚C , 2h
3	$SnCl_2.2H_2O$	PVA	Co-precipitation	350 ˚C , 2h
4	$SnCl_2.2H_2O$	–	Co-precipitation	350 ˚C , 2h
5	$SnCl_2.2H_2O$	Sucrose	sol-gel	500 ˚C , 2h
6	$SnCl_2.2H_2O$	–	Hydrothermal (120 ˚C , 12h)	–



Scheme1: XRD, SEM and photocatalytic applications of SnO_2 prepared under different conditions.

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A novel binary composite of Zr-MOF with Cu chiral for enhanced asymmetric CO_2 fixation reaction

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Keywords: Zr-MOF, Cu Chiral, CO_2 fixation, Catalyst

The emission and accumulation of carbon dioxide (CO_2) in the atmosphere contribute significantly to the greenhouse effect and global warming [1]. The rapid industrial expansion in recent years has accelerated the accumulation of this gas and its associated adverse effects. Various strategies have been explored to remove and reduce CO_2 from the atmosphere. One such approach involves using catalysts to convert CO_2 into inert compounds [2]. This reaction can yield products with biological or pharmaceutical applications. An example is the reaction of CO_2 with epoxide precursors, resulting in the formation of chiral cyclic carbonates, which are highly valuable in the pharmaceutical industry [3].

Previous studies have utilized zeolite catalysts and complexes for these reactions. Recently, metal-organic frameworks (MOFs) have gained significant attention for this application. In the present study, a zirconium-based metal-organic framework (Zr-MOF) was synthesized and composited with a chiral copper catalyst to facilitate the CO_2 fixation reaction [4]. The catalyst was characterized using techniques such as FTIR, XRD, BET, and SEM.

The results of the CO_2 fixation reaction demonstrated that this catalyst exhibits high efficiency in converting epoxides to cyclic carbonates. Additionally, the chiral selectivity of this composite was achieved with a high percentage. The findings indicate that the novel synthesis method for binary composites, previously employed for nitrogen fixation reactions, is also effective for CO_2 fixation.

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Al(OH)(PZDC): An Effective Carrier for controlled Release of Poorly Soluble NSAID Celebrex

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Keywords: Al(OH)(PZDC), Drug delivery, Celebrex, Solubility

Nonsteroidal anti-inflammatory drugs (NSAIDs) are widely used for their analgesic, antipyretic, and anti-inflammatory properties. However, many NSAIDs suffer from poor water solubility, leading to low bioavailability and gastrointestinal side effects [1]. Targeted drug delivery systems aim to overcome these challenges by enhancing solubility, stability, and site-specific delivery, thereby minimizing side effects and improving therapeutic efficacy [2].

Investigation about the controlled release of the loaded drugs into the porous materials has applications in medicine and pharmaceutics. Controllable drug delivery has been extensively used, due to its numerous advantages. According to the special surface area and suitable pore diameter, metal-organic frameworks (MOFs) could be useful to support a variety of large and small molecules [3]. The loading of drug molecules in the pores of (MOFs) and releasing at the target tissue improve the drug efficiency and reduce the dosage of it. Other benefits of nano-carriers include having the small size, reducing toxicity, improving drug solubility, stability and drug efficacy and achieving the constant therapeutic level [4].

Celebrex as a NSAID is belonged to the second class of drugs that have low solubility and permeability. It can be said that it is a hydrophobic drug [5]. Because of its low solubility, the concentration of celebrex, is measured by UV-Vis. This drug, due to the low solubility, has low biocompatibility and incomplete absorption in the gastrointestinal tract. Therefore, many attempts have been done to improve the solubility of it. As a result of this works, the solubility, biocompatibility and permeability of celebrex were increased. Because of this, metal-organic frameworks from Al(OH)(PZDC) were used as a support for it. The mechanism of in-vitro releasing is studied in simulated body fluid (without enzymes). From UV-Vis analysis, results showed that 85 percent of the insoluble drug released in SBF from the porous support which is much higher than the pure drug.

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Synthesis of size-controlled Ag nanoplate and its applications

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Keywords: Nanoparticles, Ag nanoplate, Co-precipitation

Nanoparticles are small materials with sizes ranging from 1 to 100 nm. NPs possess unique physical and chemical properties due to their high surface area and nanoscale size. Their optical properties are reported to depend on the size, which imparts different colors due to absorption in the visible region. Their reactivity, toughness and other properties are also dependent on their unique size, shape and structure. Silver nanoparticles are silver particles with a diameter between 1 and 100 nm. Although they are usually spherical, they may also have shapes such as diamonds, octahedrons, triangles, and plates. Silver nanoparticles are one of the most useful forms of heavy metals in nanotechnology applications. Silver as a quantum dot has a tunable band gap that can be controlled by changing the size and diameter of the quantum dots. Due to its extraordinary bactericidal properties, low resistance to electricity, heat and surface plasmon resonance, silver nanoparticles are used in various products including consumer goods, healthcare, catalysts, electronics, etc. Herein, the synthesis of silver nanoplate has been reported. This synthesis has been carried out using silver nitrate, sodium borohydride and H_2O by co-precipitation method. These silver nanoplates due to their unique properties can be used in electrochemical applications such as sensors, batteries, supercapacitors, etc. (**Scheme1**).

Scheme1: Synthesis of Ag nanoplates and its applications.

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Reactivity of Different Cycloplatinated(II) Complexes toward a Bisphosphine Ligand: Experimental and Theoretical Investigations

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Keywords: Cycloplatinated(II) complexes, Platinum, Biphosphine ligand, DFT calculations

Cyclometalated transition metal complexes, especially square-planar platinum(II) complexes, are gaining attention for their diverse potential applications, including photocatalysis, sensing, anticancer treatments, and optoelectronic devices [1,2]. In addition to mononuclear complexes, there is growing interest in binuclear complexes with bridging ligands, which are valuable for self-assembly, catalysis, electrical conductivity, and photoactive applications. The choice of bridging ligands is critical for enhancing electronic communication between metal centers; rod-like phosphorus-donor spacers are particularly effective due to their aligned molecular orbitals with attached metal centers. Moreover, these ligands exhibit desirable properties such as photostability, conjugation, and rigidity, which further enhance the performance of the resulting complexes.

This study presents the preparation, characterization and density functional theory (DFT) optimization of a series of binuclear cycloplatinated(II) complexes, $[Pt_2R_2(C^\wedge N)_2(\mu\text{–dppac})]$, R = p-MeC_6H_4 or Me and C^N = 2-(2,4-difluorophenyl)pyridine (dfppy) or, 2,2′-bipyridine *N*-oxide (O-bpy), dppac = 1,1′-bis (diphenylphosphino)acetylene, labeled as **1–4** (**Figure 1**). The complexes are characterized through multinuclear NMR spectroscopy (^{1}H, $^{31}P\{^{1}H\}$ and $^{195}Pt\{^{1}H\}$) and confirmed *via* single crystal X-ray diffraction. The work further discusses their geometries and electronic spectra, providing insights into their structural and electronic characteristics. Electronic structure analysis, along with DFT calculations, reveals a ^{1}MLCT(metal-to-ligand charge transfer) for **1,** while supporting a mixed L'LCT (ligand-to-ligand charge transfer)/^{1}MLCT for **2–4.**

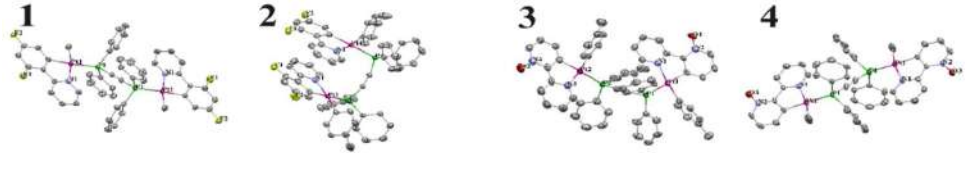

Figure 1. Molecular structures of **1-4**.

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Tetracycline phtodegradation under UV light by ZnO nanorods/BiOBr nanosheets heterojunction

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Keywords: Photocatalytic degradation, Zinc oxide, Bismuth oxybromide, Photocatalyst

The presence of antibiotics like tetracycline (TC) in water and wastewater is a global concern due to the potential harm they can cause to humans, animals, and the environment [1]. One effective method to reduce the amount of antibiotics in wastewater is through photodegradation by using photocatalysts such as zinc oxide (ZnO) [2]. In this study, ZnO nanorods were synthesized as photocatalysts using the chemical bath deposition method. To improve the photocatalytic activity and enhance the photodegradation of TC, ZnO nanorods/BiOBr nanosheets heterojunctions were synthesized at different mole ratios (Zn: Bi) using the hydrothermal method at pH=9. The structure and optical features of the heterojunction were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and UV-visible diffuse reflectance (DRS). The study of TC photocatalytic degradation results showed that the ZnO /BiOBr heterojunction exhibited higher photocatalytic activity compared to pure ZnO and BiOBr.The photodegradation rate constant (k) of ZnO/BiOBr, optimized at a mole ratio of 2:1 (Zn:Bi), was about 0.011 min^{-1}, which was significantly higher compared to pure ZnO nanorods (0.008 min^{-1}) and pure BiOBr (0.004 min^{-1}). This enhancement was attributed to the inhibition of charge carrier recombination, leading to a reduction in the recombination rate of electron-hole pairs. Also, a comparison between different samples demonstrated that the composite with a mole ratio of 2:1 (Zn: Bi) has the highest degradation efficiency. Overall, the photocatalytic degradation process showed improvement, with the degradation efficiency increasing from 62.55% for ZnO to 68.84% for ZnO/BiOBr at a ratio of 2:1.

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Preparation of lithium cobalt oxide compounds for use in lithium-ion batteries

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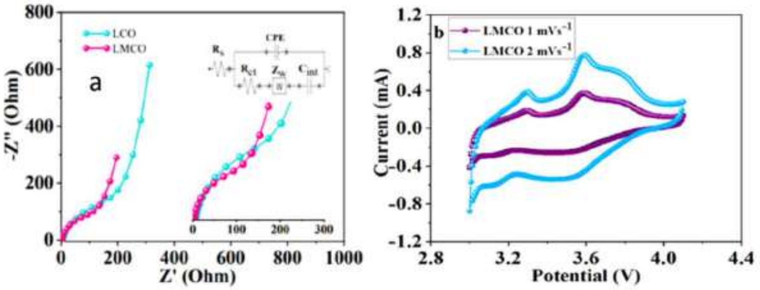
Keywords: Lithium cobalt oxide, Cathode, Lithium-ion battery, Electrochemical performance, Cyclic voltammetry

Lithium cobalt oxide (LCO) is widely used in lithium-ion batteries due to its high volumetric energy density, which is generally charged up to 4.3V. This cathode has revolutionized portable electronics such as cell phones and laptop computers, but the high cost, toxicity, chemical instability in deep charge, and safety concerns associated with lithium cobalt oxide prevent its use for transportation and storage applications. Constant prevents. In addition to the inherent instability of lithium cobalt oxide at high voltage, the interaction between the lithium cobalt oxide composition and other battery components is another challenge[1,2]. In this thesis, LCO, LMnCO(lithium manganese cobalt oxide) , LSrCO(lithium strontium cobalt oxide) and LZnCO(lithium zinc cobalt oxide) cathode materials were synthesized by sol-gel method. Synthetic materials were identified by X-ray diffraction analysis (XRD) and Fourier-transform infrared spectroscopy (FT-IR) analyses. Then, cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) tests were used to us these materials in batteries. For this purpose, first in 1 M $LiNO_3$ aqueous electrolyte, cyclic voltammetry test of LCO, LMCO, LZnCO, LSrCO, LNiCO(lithium nickel cobalt oxide), LMgCO(lithium magnesium cobalt oxide) samples had currents of 6.53 and 60.08, 7.79, 6.57, 174.58 mA h. which have a capacity of about 26.11, 158.09, 25.11, 21.91, 69.95 and 145.48 $mAhg^{-1}$. In the last stage, LCO and LMnCO samples which had better capacity in organic electrolyte system were examined by cyclic voltammetry and impedance test, and the capacity of LCO and LMnCO was 83.27 and 214.06 $mAhg^{-1}$, respectively. The reason for this is the presence of Mn element in the structure of LCO **(Scheme1)**.



Scheme1: (a) Nyquist curve of LCO and LMCO electrodes, (b) Cyclic voltammetry graphs LMCO at scan rates of 1 mV/s

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External field effect on some optoelectronic properties of keto and enol Guanine conformers

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Keywords: Guanine, Keto/Enol conformers**,** TD, Optolectronic, UV spectrum

Conductive molecular structures such as Guanine-like structures have many applications in molecular electronics [1]. For the control heat-electric interfere in molecular opto-nanoelectronic field-effect devices, details of the charge and energy transfer mechanisms in these molecular systems under external electric field (EF) should be known. Therefore, in this paper, the external electric field (EF) effects on some Optolectronic properties of the keto and enol Guanine conformers are studied, using time-dependence density functional theory (TD), at UB3LYP/6-311G level of theory. Sample of these results are shown in **Table 1** and **Figure 1**. Analysis of the calculated results shows that the response of these two molecular conformers (keto and enol) to the EF is completely different. This response difference can be caused by the way the π-conjugated bonds in these conformers are extended due to the application of an external EF. Analysis of these results also showed that the electrical conductivity of the keto conformer is higher than that of the enol conformer. This issue can be due to the decrease in the E_{gap} of the keto conformer due to the application of the EF.

Table 1. The external EF effect on E_{gap} (E_{HOMO}-E_{LUMO}) of the Guanine conformers

	Keto	**Enol**
EF (10^{-4}au)	E_{gap}	E_{gap}
0	8.21	7.76
20	8.18	7.92
80	7.46	8.03
100	7.13	8.06

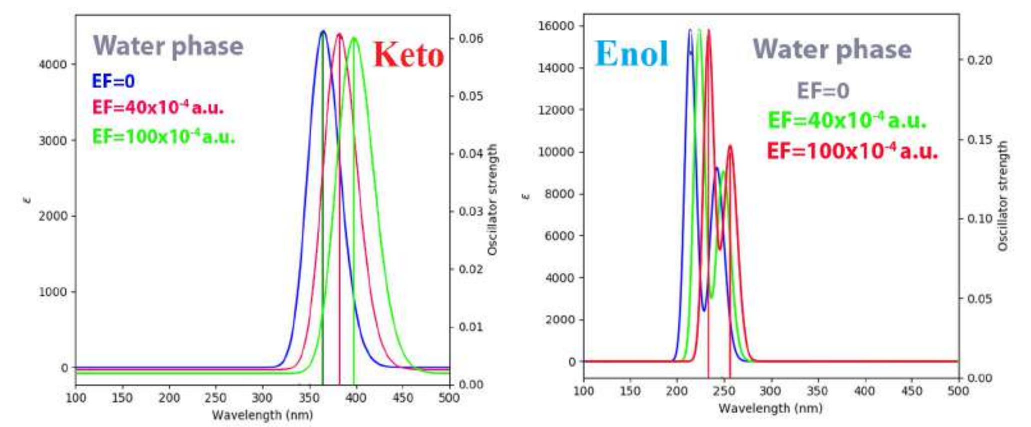

Figure 1. The external EF effect on UV spectra of the Guanine conformers.

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Investigation of electrochemical hydrogen storage capacity in PAN-GO@TiO_2 nanofibers

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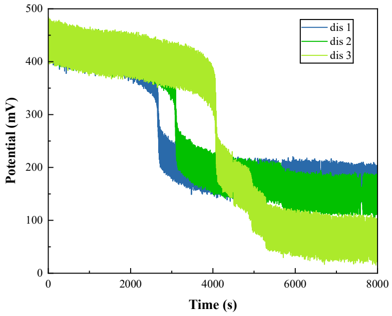
Keywords: Hydrogen storage, Nanofiber, Electrospinning, Electrochemical

Today, environmental pollution and energy shortages pose significant challenges for the future of our planet. Consequently, adopting technologies based on renewable energy sources is crucial to addressing the pollution resulting from non-renewable fossil fuels. Hydrogen, with its high energy content and abundance, emerges as an ideal energy carrier for this purpose. [1]. Physical storage of hydrogen on the surface of porous materials such as nanofibers (NFs) is one of the main methods for use in vehicles. In recent years, hydrogen storage by NFs has received worldwide scientific and technological attention. NFs are one of the most important components of nano technology that can be used in many different fields [2]. Energy production and storage sources, water and environmental treatment, healthcare and medicine, are very diverse areas in which these structures can be used. NFs are suitable for many important applications due to having properties such as a very high surface-to-volume ratio compared to other known materials [3]. In this study, PAN-GO@TiO_2 NFs were prepared by electrospinning method, and the electrochemical storage capacity of hydrogen in the prepared NFs was investigated. Hydrogen storage capacity in the studied NFs was 222.22 mAh/g. The discharge of PAN-GO@TiO_2 NFs can be seen in the current of 2 mA (**Scheme1**).



Scheme1: Discharge of PAN-GO@TiO_2 NFs at a current of 2 mA.

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Synthesis and Characterization of a Cyclometalated Platinum(II) Complex with a Biologically Phosphine Ligand

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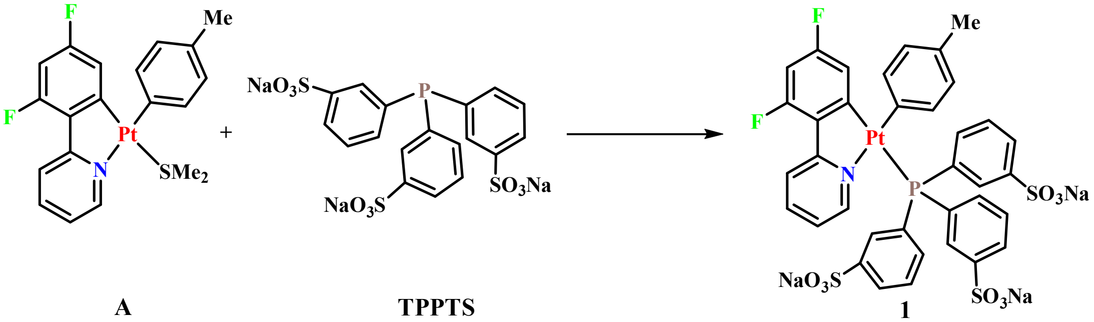
Keywords: Phosphine ligands, Cycloplatinated(II) complexes, Biological activity.

The use of cycloplatinated (II) complexes in cancer research is becoming more and more popular [1]. Strong σ(Pt–C) bonds in these complexes enhance their stability under physiological settings, preventing off-target reactions and, hence, simplifying possible therapeutic uses [2]. The ultimate emissive behavior and the cytotoxic activity of the Pt are significantly influenced by the choice of auxiliary ligands and the cyclometalated group, for which subtle alterations might have a significant impact on the biological effect [3]. Herein, we present the synthesis and characterization of a cycloplatinated complex [Pt(*p*-MeC$_6$H$_4$)(dfppy)(TPPTS)], **1**, (**Scheme 1**) that contains a water-soluble phosphine triphenylphosphine 3,3',3''-trisulfonate (P(C$_6$H$_4$SO$_3$Na)$_3$; TPPTS) as an auxiliary group and a cyclometalated ligand, 2-(2,4-difluorophenylpyridine, dfppy. This system was designed by considering several features that make the complex interesting for biological studies.



A **TPPTS** **1**

Scheme 1. Synthetic route for the preparation of **1**.

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Catalytic application of metal-organic frameworks based on copper in the synthesis of *N*-heterocyclic compounds

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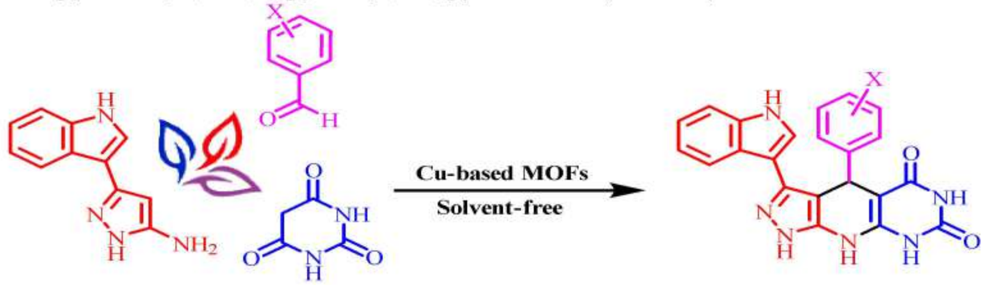
Keywords: Metal-organic frameworks (MOFs), Multicomponent reactions, Heterocyclic compounds.

In recent decades, metal-organic frameworks (MOFs) have experienced exponential growth. This class of crystalline hybrid materials, composed of metal canters and organic ligands, offers unique chemical versatility, a customizable framework, and exceptionally large and permanent internal porosity [1]. MOFs possess a high surface area, significant porosity, and the ability to chemically adjust through the modification of organic ligands, enhancing their efficacy as adsorbents and catalysts. The selection of an appropriate synthetic route plays a crucial role in designing MOF materials with specific sizes, morphologies, and nanostructures [2]. Biological based structure such as *N*-heterocyclic scaffold compounds have been considered as candidates for the design and discovery of new biologically active compounds. It is very important to supply new and easy methods for the preparation of target compounds with unique features. In this regard, 1,4-dihydropyridine structures containing indole, pyrazole and pyrimidine moieties are suitable candidates for biological and pharmacological purposes [3]. In this project, we have tried to use the catalytic application of Cu-based MOFs for the synthesis of pyrazolo[4′,3′:5,6] pyrido[2,3-d]pyrimidines (**Scheme**).



Scheme: Synthesis of pyrazolo[4′,3′:5,6] pyrido[2,3-d]pyrimidines using Cu-MOFs.

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DFT design of novel nano-bud from $B_{12}N_{12}$ and nanobowl

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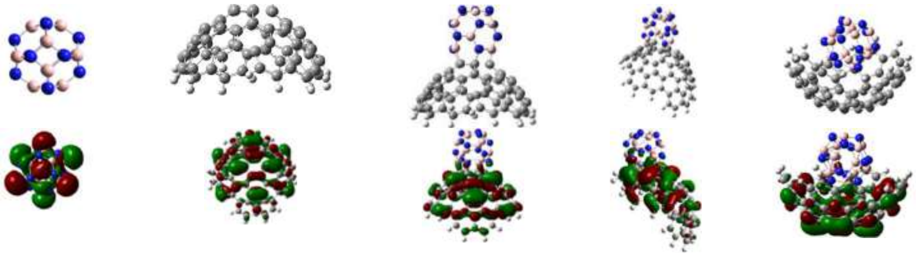
Keywords: Nanobud, Nanobowl, $B_{12}N_{12}$, DFT, Molecular Design

Recently, the idea of nanoparticle hybridization and improving their properties by forming nanobuds has been used, and it has been tried to design nanoparticles with improved properties by combining fullerenes with different size [1,2].In this research, by grafting $B_{12}N_{12}$ nanocluster on nanobowl, new structures of nanobuds were designed and the possibility of forming these nanobuds was investigated using DFT calculation methods. For this purpose, optimization of the structure.The energies of HOMO and LUMO frontier orbitals and Eg values were calculated using DOS spectra and showed that the designed nano-buds have better electrical properties than the parent molecules. Calculating the contribution of the dispersion term in the energy of the nanobuds showed that compared to the parents, larger dispersion energy was obtained for the designed nanobuds. In this study, all calculations were perform using the Gaussian 09W packag [3].The geometry of molecules was optimized using B3LYP functional method, DFT method and 6-311G(d,p) basis set [4].The electronic density of state (DOS) of the molecules, which represents the electrical properties, was obtained with the Gauss Sum program (**Scheme1**).



Scheme1: DFT design of novel nano-bud from B12N12 and nanobowl

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Synthesis, characterization and structural analysis of hetero-metallic trinuclear copper(II)–cadmium(II) complex derived from a Salen-type ligand

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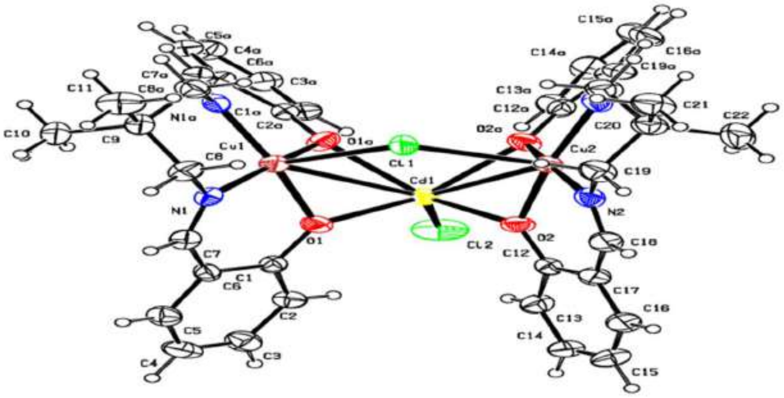
Keywords: Hetero-metallic, trinuclear, Copper(II)-Cadmium(II), Salen ligand

The new trinuclear hetero-metallic copper(II)-cadmium(II) complex, $[Cu_2(\mu\text{-}L)_2CdCl_2]$, has been synthesized using [CuL] as a so-called ‘‘ligand complex’’ (where L^{2-} = N,N'-bis(salicylidene)-2,2-dimethylpropylenediaminato) and structurally characterized. Crystal structure analysis reveals that complex contains a trinuclear moiety in which two [CuL] units are bonded to a central cadmium(II) ion through double phenoxido bridges. Complex contains a heterotrinuclear $[Cu^{II}Cd^{II}Cu^{II}]$ unit in which the central cadmium ion is connected to two copper(II) centers through two doubly bridging phenolate oxygen atoms in addition to a terminal chloride ion. On the other hand, the Cd(II) ion in complex adopts distorted square pyramidal (CdO_4Cl) geometries (**Scheme1**).



Scheme1: ORTEPdiagram for the complex $[Cu_2(\mu\text{-}L)_2CdCl_2]$ showing the atom labeling.

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Synthesis, characterization and structural analysis of hetero-metallic dinuclear copper(II)–mercury(II) complex derived from a Salen-type ligand

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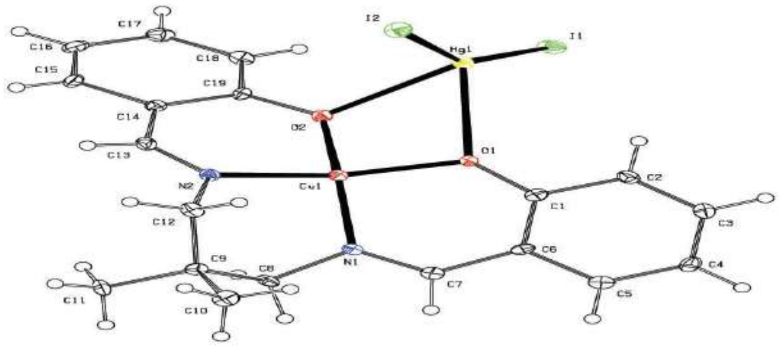
Keywords: Hetero-metallic, Dinuclear, Copper(II)- Mercury(II), Salen ligand

The new dinuclear hetero-metallic copper(II)-mercury(II) complex, $[CuL\{HgI_2\}]$, has been synthesized by reacting [CuL] as a so-called ‘‘ligand complex’’ (where H_2L = N,N′-bis(2-hydroxyphenylidene)-2,2′-dimethyl-1,3-propanediamine) with HgI_2. The complex has been characterized using elemental analysis, IR spectroscopy and X-ray diffraction. Structural studies on complex reveals the presence of a heterodinuclear $[Cu^{II}Hg^{II}]$ unit in which the central Cu(II) and Hg(II) ions are connected to each other by two phenolate oxygen bridges. In this complex, the Cu(II) ion adopts a distorted square planar (CuN_2O_2) geometry while the Hg(II) ion in complex adopts tetrahedral (HgO_2I_2) geometries (**Scheme1**).



Scheme1: ORTEPdiagram for the complex $[CuL\{HgI_2\}]$ showing the atom labeling.

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Optimizing Supercapacitor Performance: A Study on Polypyrrole Electrodeposition on Carbon Fibers

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Keywords: carbon felt, flexible supercapacitor, polymer materials, binder-free electrode

Polypyrrole (PPy) as a pseudocapacitive electrode material is an ideal candidate for the fabrication of ASCs. PPy was electrodeposited on CF in the electrolyte solution containing 173 μL pyrrole monomer and 0.1 M sodium chloride by applying a constant potential of +0.8 V (vs. Ag/AgCl) for 700s [1]. The FE-SEM images of PPy@CF show a rough globular morphology (Fig. 1a, b). As can be observed, the surface of carbon fibers is covered with a large number of particles that are densely connected. The EDX mapping and spectrum show the presence of carbon, nitrogen, and oxygen elements in the PPy@CF electrode (Fig. 1c, d). The electrochemical investigations of the prepared materials for the negative fiber electrode were performed in a 3M KOH electrolyte in a three-electrode cell configuration. The CV and GCD curves of the PPy@CF electrode under various scan rates and current densities are shown in Fig. 1e and f, respectively. The quasi-rectangular shape of the CV curves and nonlinear quasi-triangular charge/discharge plots show pseudo-capacitance behavior of PPy@CF electrode. The maximum areal specific capacitance calculated using the discharge curve for the PPy@CF electrode is found to be 259.6 mF cm^{-2} at 1 mA cm^{-2} (Fig. 1g). The Nyquist plot predicts fast charge transfer in the PPy@CF electrode (Fig. 1h).

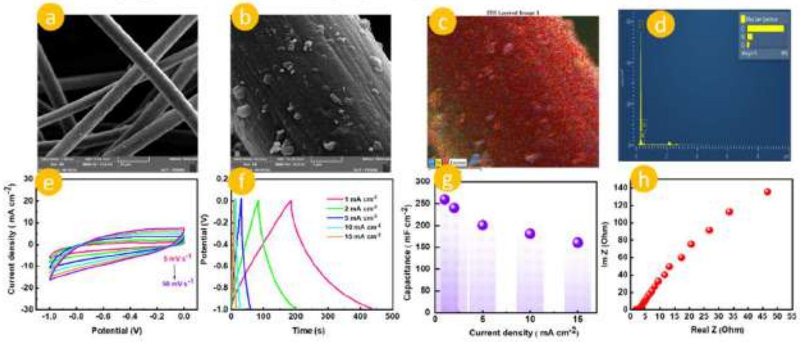

Fig. 1: FE-SEM of PPy@CF (a, b), EDX mapping images (c), spectra (d) of PPy@CF, CV curve of PPy@CF electrode at various scan rates (e), GCD curve of PPy@CF electrode at various current densities (f), Rate capability (g), Nyquist plots of the PPy@CF electrode at open circuit potential (h).

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Investigation of catalytic activity of modified natural zeolite in water oxidation

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Keywords: Natural zeolite, Water oxidation, Heterogeneous catalyst, Oxygen production

The depletion of nonrenewable natural fossil fuel resources from the earth has become a major global concern. Thus, a major stream of the research trend during the last decade has deviated towards the development and search for alternate sustainable energy sources. The oxygen evolution reaction (OER) of water splitting is essential to electrochemical energy storage applications [1,2]. The energy required for the catalytic process of water oxidation is diminished by the presence of metals in higher oxidation states. In this study, we report the synthesis of modified natural zeolite with Mn, Co and Ni by ion exchange and laser ablation in liquid (LAL) methods. The compounds were characterized by FTIR, XRD, EDS and FE-SEM. Observed results showed that the water oxidation activity of the modified natural zeolites in the presence of ammonium Ce(IV) nitrate were higher than that of natural zeolite. The oxygen production rates in the presence of catalysts were found to be in an order of Mn/zeolite > Co/zeolite > Ni/zeolite > natural zeolite.

Schem 1. Natural zeolite (a), Co/Zeolite (b), Mn/Zeolite (c), Ni/Zeolite (d), Ni/Zeolite (LAL) (e), Mn/Zeolite (LAL) (f) as the catalysts.

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Clay-Based Nanocomposites as Eco-friendly Materials for Electrochemical Hydrogen Storage

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Keywords: Montmorillonite K10, Hydrogen storage, Nanocomposites, Electrochemistry, Chemical synthesis

Clay is an important natural substance. With a better understanding of clay structure, montmorillonite may be used in more components and products for catalysis, food additives, antibacterial action, polymers, sorbents, etc. Clay-based materials are promising for energy conversion and storage[1, 2].

Recent years have seen hydrogen energy consumption increase. Clean, safe, and adaptable hydrogen helps decarbonize transport. Renewable energy development improves energy efficiency and decarbonizes the system. Hydrogen's non-toxicity, quantity, and ease of preparation make it an intriguing fuel[3, 4].

This study presents the innovative implementation of clay-based nanocomposites for the purpose of hydrogen storage. The Li-Co-Mn double spinel was synthesized using the combustion technique using carboxylic acid as both the fuel and chelating agent. This double spinel compound was employed as the electrocatalyst in this study. The produced samples were analyzed using different methods including XRD, EDS, and SEM to determine their purity and morphology. This study investigates the hydrogen storage capacity of nanocomposites manufactured using chronopotentiometry charge-discharge procedures. The results suggest that the incorporation of Li-Co-Mn spinel oxide nanoparticles into the clay layers leads to an increase in discharge capacity, representing a greater capacitance compared to pure clay. The findings of our study suggest that the use of Li-Co-Mn spinel oxide nanoparticles for modification has potential as an economical approach to enhance the electrochemical performance of clay-based materials.

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Electrode material based on sol-gel synthesized Ca-Mn-O nanostructures for electrochemical hydrogen storage application

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Keywords: Sol-gel Synthesis, Nanostructures, Hydrogen storage

The growing demand for efficient and sustainable energy solutions has intensified the exploration of advanced materials for hydrogen storage[1]. In this study, we investigate the potential of calcium-manganese oxide (Ca-Mn-O) nanostructured materials as a high-capacity hydrogen storage. Ca-Mn-O nanostructures are synthesized using a sol-gel method, yielding highly porous, high-surface-area materials, ideal for gas adsorption applications. Also, amino-acids is chosen as the best fuel and capping agent, resulting in the production of manganate materials. In order to compare the generated samples' surface area, magnetic properties, purity, and structural, chemical, and physical characteristics with one another.

Including Structural and morphological analysis reveals the formation of well-defined nanoscale architectures, which enhance hydrogen adsorption through both physisorption and mechanisms. Through the use of the CV and CHP techniques in a three-electrode cell with a 2.0 M KOH electrolyte, the potential of Ca-Mn-O materials for electrochemical energy storage was examined. By applying advanced characterization techniques such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray diffraction (XRD), this project will offer in-depth insights into the composition-structure-morphology-performance relationships of hydrogen storage[2]. The results demonstrate that Ca-Mn-O nanostructures exhibit improved hydrogen uptake compared to bulk materials, attributed to their surface chemistry and pore distribution. These findings suggest that Ca-Mn-O nanostructures hold promise as efficient, cost-effective hydrogen storage materials, contributing to the advancement of hydrogen-based energy systems.

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Investigating the optimal percentage of MXene as a conductivity enhancer in lithium-ion batteries

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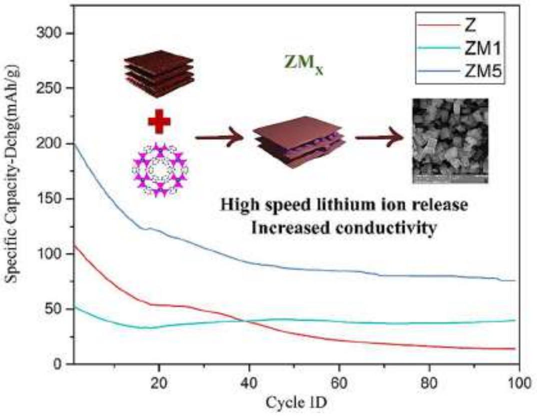
Keywords: MXene, Lithium-ion battery, Conductivity

In this study, with the help of in situ synthesis, first Zif was synthesized in ammonia environment and then it was composited with optimal percentages of MXene (Ti_3C_2) with the help of ultrasonic bath. Scanning electron microscope images confirm the successful synthesis of this compound. MXene with two-dimensional structure increases the conductivity and Zif with specific pore diameter and regular network makes the path of lithium diffusion uniform and accelerated. As a result, the synthesized anode presented a reversible capacity of 149 mAh/g after 100 cycles at a current of 0.1 and a 27% capacity reduction compared to the initial capacity. Synthetic composites as anode materials in lithium-ion batteries show excellent durability and high specific capacity (**Scheme1**). [1,2]



Scheme1: A novel Zif @MXene-based composite demonstrated superior lithium storage as an anode for lithium-ion batteries (LIBs).

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Oxidative Addition of Iodomethane to a Diarylplatinum(II) Complex: Synthesis, Characterization and Theoretical Elucidation

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Keywords: Organoplatinum, Oxidative addition, Nitrogen donor ligands

In many chemical processes, including homogeneous catalysis and biology, oxidative addition reactions involving square planar complexes of d^8 metal ions, such as Pt(II), are essential. [1]. Extensive mechanistic investigations have shown that these compounds often progress through an S_N2 pathway [2]. In this study, the oxidative addition reaction of diarylplatinum(II) complex $[\mathrm{Pt}(p\text{-}\mathrm{MeC_6H_4})_2(N\text{-}\mathrm{PhPhen})]$, **1**, *N*-PhPhen = phosphine *N*-phenyl-1,10-phenanthroline-2-amine, with MeI led to the formation of *trans*-$[\mathrm{PtMeI}(p\text{-}\mathrm{MeC_6H_4})_2(N\text{-}\mathrm{PhPhen})]$, **2** (**Figure 1**). The new Pt(II) and Pt(IV) complexes were characterized by NMR spectroscopy and single crystal X-ray crystallography. The theoretical aspects of the mechanism for the oxidative addition reaction were also studied by density functional theory (DFT) calculations.

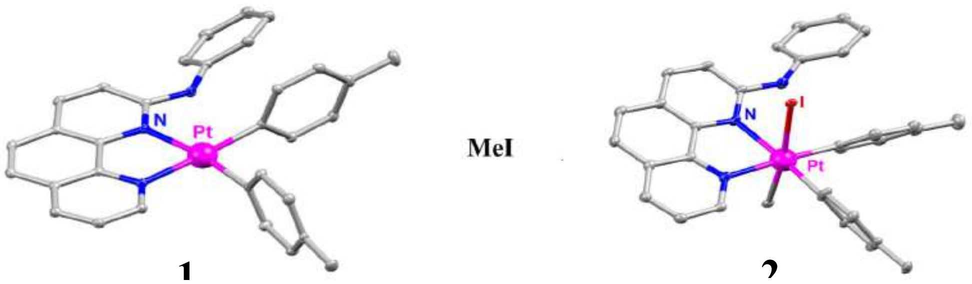

Figure 1. Oxidative addition process for the preparation of **2**.

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Thermal degradation of kerosene in water by nano ZrO_2 as catalyst

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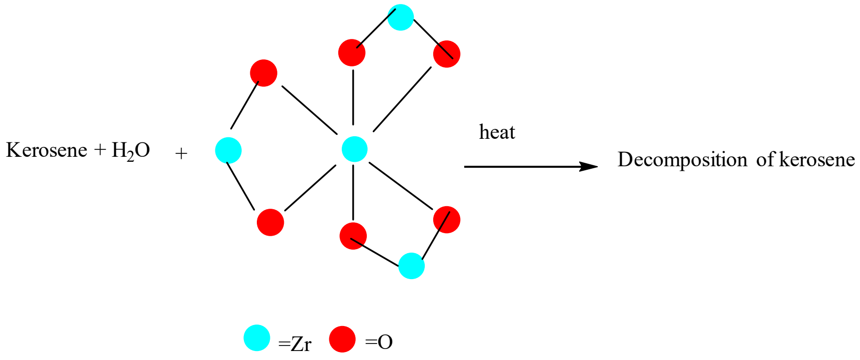
Keywords: Kerosene, Nano ZrO_2, Thermal degradation

Kerosene is a liquid mixture of hydrocarbons (n-alkanes, cycloalkanes and some aromatic compounds) that can be produced by the fractional distillation of crude oil [1]. This compound is a cause poisoning common and sometimes reason of morbidity and mortality in different age groups. Produced of petroleum and transfers of its may be caused to pollution of water that are highly hazardous to aquatic living and human being [2]. According to data reported in 2020, ZrO_2 under thermal condition at 300-673 k led to generation of hydroxy radical [3]. So, in this study, degradation of kerosene in water was study by nano ZrO_2 catalyst under thermal condition and data were compare with ASTMD2163 test (**Scheme 1**).



Scheme1: Decomposition of kerosene by nano ZrO_2

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Removal of methylene blue textile pollutant from wastewater using magnetic composite

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Keywords: Metal-organic framework ternary composite, Methylene blue, Adsorption

Textile industry wastewater containing hazardous nature, non-biodegradability as well as toxic and complex compounds causes serious problems in human, plant, and animal ecosystems [1,2]. There are several methods to purify wastewater from pollution, with adsorption being a widely recognized and efficient technique due to its simplicity, effectiveness, cost-effectiveness, and potential for recovering and reusing the adsorbent [3]. In this research, a magnetic ternary composite of the Zeolitic imidazolate framework was synthesized as an adsorbent and evaluated its effectiveness for dye removal [4]. Various factors influencing adsorbent performance, including the initial amount of adsorbent, dye concentration, contact time, pH, and the recovery and reuse of the adsorbent were investigated. SEM, FT-IR, and XRD were utilized to identify the adsorbent structure. The equilibrium isotherms were assessed using the Langmuir, Freundlich, and Temkin models. The ternary composite was aligned with the Temkin model. The adsorption kinetics were examined using the pseudo-first-order and pseudo-second-order models, along with the intraparticle diffusion model. Results indicated that the kinetics conform to the pseudo-second-order model.

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Synthesis, Characterization, and Investigation of the Antibacterial Properties of the Asymmetric Tridentate Schiff Base Ligand (ONO) and Its Nickel Complex

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Keywords: Schiff Base, Nickel(II), Tridentate, Synthesis

The desired ligand was formed from the condensation reaction of 2-methyl-3-aminoquinazoline and 5-bromo-3-hydroxybenzaldehyde, resulting in the Schiff base ligand 5-bromo-2-hydroxy-3-methoxybenzylideneamino-2-methylquinazoline. The synthesized ligand belongs to the category of tridentate ONO ligands [1].

The ligand reacted with Nickel(II) ions in the presence of pyridine and was identified using various methods including FT-IR spectroscopy, elemental analysis, mass spectrometry, electrical conductivity, and melting point determination. Also the synthesized complex and free ligand were screened for their antibacterial activities against Four bacterial strains and showed antibacterial effects [2]. The results indicated that the complex exhibited greater antibacterial activity compared to the free ligand. (**Fig. 1**).

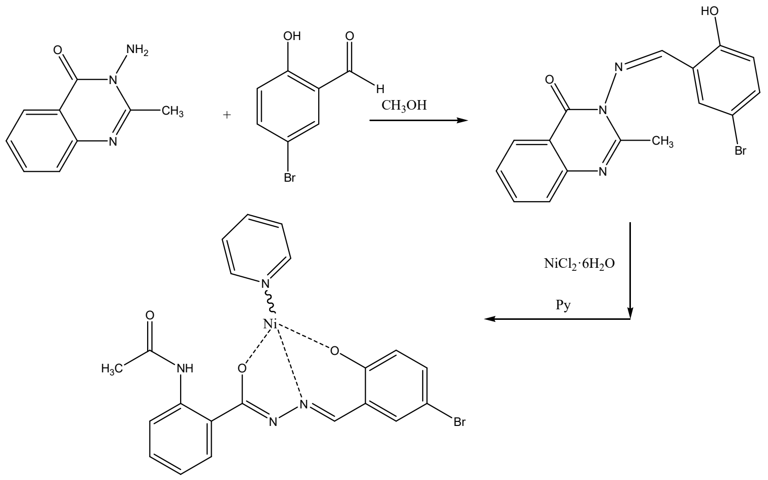

Fig. 1: Synthesis of free ligand and its comlex.

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Coconut Shell-Based Activated Carbon: Synthesis, Characterization, and Adsorption Capacity for Iron (III) Ions

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Keywords: Active Carbon, Fe(III), Efficient Adsorption, Coconut Shell

Activated carbon is widely used for the removal of pollutants from water due to its high surface area and adsorption capacity.Coconut shell is a renewable and abundant agricultural waste material that can be used as a precursor for the production of activated carbon.

This study focuses on the production of activated carbon from coconut shell and its application for the adsorption of iron (III) from aqueous solutions. Activated carbon was produced from coconut shell using physical activation. The prepared activated carbon was characterized using FTIR, BET, and SEM analyses. Batch adsorption experiments were conducted to study the removal of iron (III) ions from aqueous solutions. The effects of initial iron concentration, pH, adsorbent dose, and contact time were investigated.

The activated carbon produced from coconut shell exhibited a high degree of microporosity and a large surface area, as indicated by the high iodine number.The activated carbon had lower dust content and higher strength and hardness compared to other types of activated carbon.

The adsorption of iron (III) ions was found to be optimal at an initial concentration of 100 ppm, pH 5.5, adsorbent dose of 2.5 g, and contact time of 80 minutes. Adsorption isotherms were best described by the Langmuir model, suggesting monolayer adsorption on a homogeneous surface.Adsorption kinetics followed the pseudo-first-order model, indicating that the rate-limiting step is the diffusion of the adsorbate into the pores of the adsorbent.

Activated carbon produced from coconut shell showed excellent adsorption capacity for the removal of iron (III) ions from aqueous solutions.

The adsorption process was influenced by various parameters such as initial concentration, pH, adsorbent dose, and contact time. The adsorption isotherms and kinetics models provided insights into the adsorption mechanism and the rate-controlling step. The findings suggest that coconut shell-based activated carbon can be an effective and low-cost adsorbent for the treatment of iron-contaminated water.

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NO_2 detection and elimination using S-doped h-BN surface

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Keywords: S-doped h-BN; NO_2; Sensing, Removal; DFT study

Despite the exceptional chemical and thermal stability of h-BN monolayer, the high bond gap energy (E_g) limits its potential applications. Therefore, efforts have been made to modify the surface characteristics through doping or decorating with different atoms. Previous experimental research has confirmed the beneficial impact of surface S-doping in this context [1]. Among various nitrogen oxides, NO_2 radical is particularly dangerous because it plays a significant role in the ozone formation in the troposphere, in the occurrence of acidic rain, reduction of visibility in the atmosphere, acidification, and eutrophication of surface waters [2]. In this work, adsorption behaviour, sensing, and removal capability of pristine and S-doped h-BN surfaces for a NO_2 molecule were investigated using DFT calculations. The generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) functional was used to calculate the exchange-correlation energy, employing TNP as the basis set. In addition, Grimme's DFT-D2 method was applied to correct for long-range Van der Waals (VdW) interactions. Based on the calculations, the NO_2 radical has a stronger interaction with S-doped h-BN than with pristine h-BN. The adsorption energies of this radical onto the h-BN, S_B, S_N, and S_{BN} surfaces were determined to be -0.29, -2.30, -3.61, and -0.33 eV, respectively. The percentage of bandgap changes ($\%\Delta E_g$) due to the adsorption process on both pristine and S-doped h-BN surfaces indicates their strong sensing ability for the NO_2 molecule. According to the results, the S_{BN} surface can be considered an excellent NO_2 sensor with a suitable recovery time (Table 1 and Figure 1). However, S_N and S_B nanosheets can be used as disposable sensors for this gas. Furthermore, they can be very effective as adsorbents for NO_2 removal.

Table 1: NO_2 adsorption energy on the pristine and S-doped h-BN surfaces, and the percentage change in the band gap energy ($\%\Delta E_g$)

System	E_{ads} (eV)	$\%\Delta E_g$
NO_2-h-BN	-0.29	84.5
NO_2-S_B	-2.30	192.7
NO_2-S_N	-3.61	355.6
NO_2-S_{BN}	-0.33	90.6

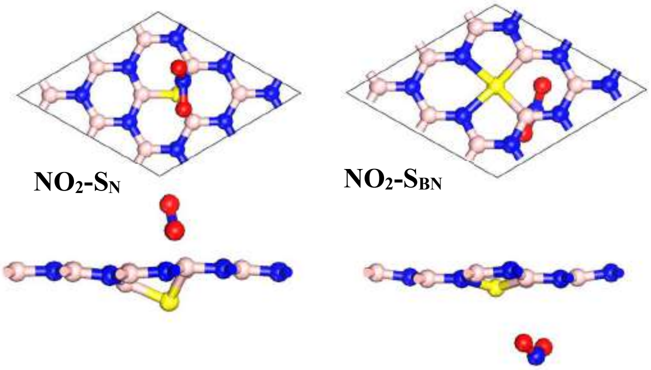

Figure 1. Optimized structures of the NO_2-S_N and NO_2-S_{BN}

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Eco-Friendly Chitosan-Based Metal-Organic Framework Composite for Organic Contaminant Degradation in Water

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Keywords: Chitosan /metal-organic framework composite, Green synthesis, Photocatalyst, Organic pollutant degradation, Water

The high aromatic compound content and complex components make it challenging to purify organic wastewater using traditional methods, leading to significant research on suitable treatment technologies [1]. Photocatalytic oxidation as an advanced technology is a promising choice in this field. The radicals resulting from this process can destroy organic pollutants and ultimately produce H_2O and CO_2 [2]. The chitosan/metal-organic framework composite has been synthesized in this research through a simple and green approach. Then, the photocatalytic capabilities of the resulting composite effective in degrading organic pollutants in water have been evaluated. The investigations revealed the first-order kinetics for pollutant degradation. The composite has provided good stability and performance after five reusability [3].

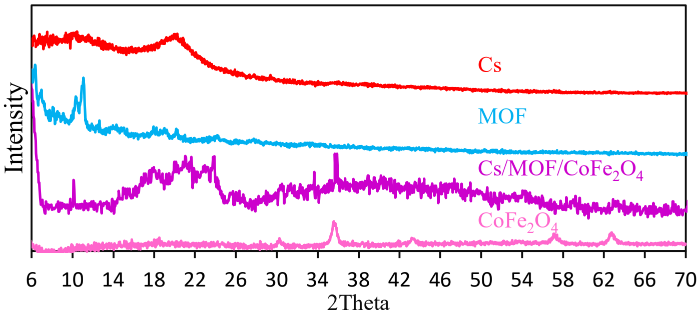

Fig 1. XRD patterns of synthesized materials

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Green synthesis of silver nanoparticles by using *Curcumin* extract

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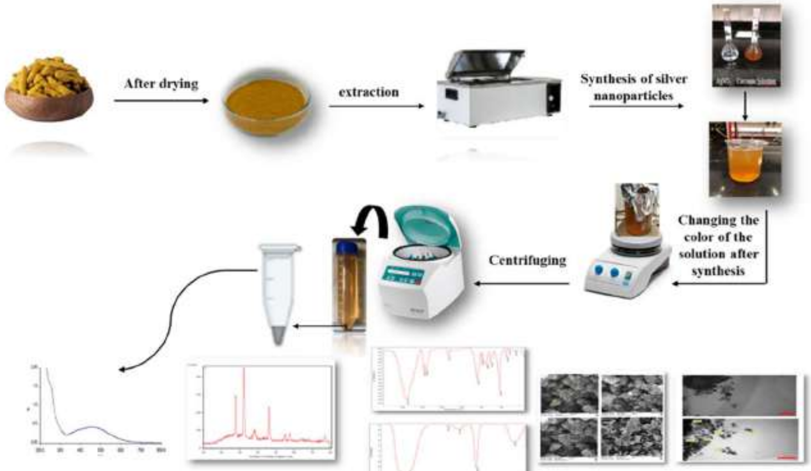
Keywords: Silver nanoparticles, Green synthesis, Maceration, FESEM, *Curcumin*

Plants have a high capacity to regenerate metals through their metabolic pathways and the biosynthesis of nanoparticles. Silver nanoparticles were synthesized using curcumin. A UV-Vis spectrophotometer determined the formation of nanoparticles and the optimization of synthesis parameters. Their size, structure, morphology, and energy dispersive spectroscopy were analyzed using FT-IR, XRD, SEM, and TEM. Synthesized silver nanoparticles were brown and reddish, and the UV-Vis spectrophotometer results were optimal in the range of 432 nm. The results of FT-IR showed the chemical compounds and functional groups of Phenol and flavonoids which are responsible for the formation of nanoparticles. The shape of spherical and rod particles, their particle size is about 21nm. Curcumin can convert Ag+ ions into nanoparticles. In addition, the synthesized silver nanoparticles have antioxidant properties.



Scheme 1: Graphical abstract of the green synthesis process of AgNPs from P. aviculare L.

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Synthesis and characterization of starch phosphates

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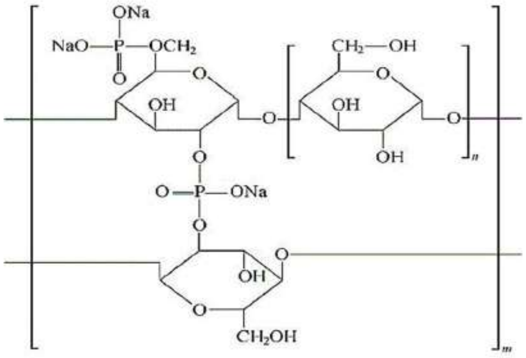
Keywords: Starch phosphates, Phosphorylation, Sodium trimetaphosphate.

Starch is a nontoxic, cost-effective, renewable, and available resource, making it invaluable in industries such as paper, packaging, food, biofuels, textiles, and others. So for environmental reasons, starch is an important industrial raw material [1]. Natural starch has certain limitations such as low shear resistance, high-temperature resistance, and high recovery trend. Also, it does not have the ideal performance for specialized applications, limiting the use of starch in some industries. Modifying natural starch particles profoundly alters its viscosity, gelatinization, and other properties, therby improving the performance of starch. Modified starches such as starch phosphates are important products with manifold properties which are used as additives in food and non-food applications [2].

In this study, a mixture of sodium tripolyphosphate (STPP) and sodium trimetaphosphate (STMP) was used in the modification process at room temperature and starch was phosphorylated.



Scheme1: The structure of starch phosphate

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Green Synthesis of COF/MOF Hybrid for Targeted Adsorption of Organic Contaminants from Water

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Keywords: Covalent-organic Framework/metal-organic framework hybrid, Green synthesis, Adsorption, Organic pollutant, Water

The discharge of organic pollutants resulting from industrial, agricultural, and urban activities poses serious risks to aquatic ecosystems, as well as to living organisms and humans [1]. A variety of physical, biological, and chemical technologies have been employed to effectively manage these pollutants. Among these methods, adsorption stands out as a straightforward and non-toxic approach, offering minimal environmental damage [2]. A melamine-based covalent-organic framework/metal-organic framework (MIL(Fe)) composite was synthesized with a green approach utilizing water as solvent. The efficacy of the composite in removing organic pollutants (Tetracycline and Congo red), from aqueous solutions was evaluated [3]. The studies indicated that the adsorption process adheres to pseudo-second-order kinetics and follows the Freundlich isotherm.

The composite demonstrated good stability and maintained its performance over three reuse cycles.

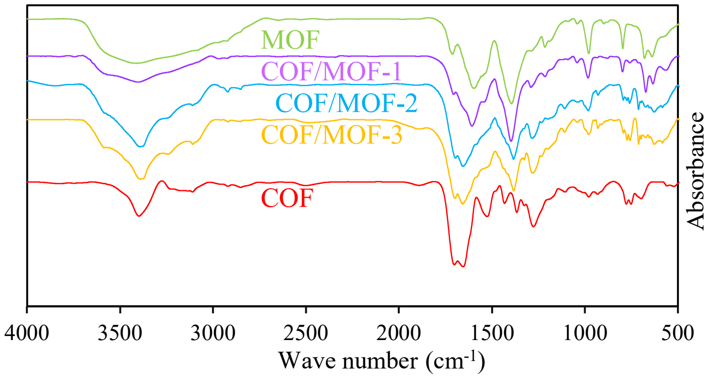

Fig 1. FTIR spectra of synthesized materials

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Synthesis and Characterization of New Schiff Base Ligands Containing Diphenyl Phosphine Group

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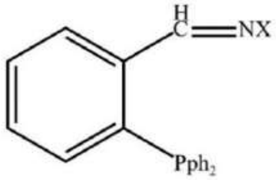
Keywords: Schiff Base, Phosphine, Amine, FT-IR, Spectroscopy

Schiff bases show one of the most important classes of ligands in metal coordination chemistry [1]. Schiff bases have wide applications in food and dye industries, analytical chemistry, catalysis, fungicidal, agrochemical and biological activities [2]. Moreover, Schiff bases are used for synthesis of metal complexes due to their easy formation and strong metal-binding ability [3]. In this work, we reported the synthesis of new Schiff base ligands containing diphenyl phosphine group. These Schiff base ligands were synthesized by the reaction of different amines containing cyclohexane and aldehydes containing diphenyl phosphine groups with 1:1 molar ratio in ethanol at room temperature for 48 hours. The solution of ligands was left to stand for a night. The precipitate was washed with n-hexane and diethyl ether and then dried in vacuum at room temperature. The structure of synthesized ligand was characterized by different methods such as UV-Vis, FT-IR and 1H NMR spectroscopies and elemental analysis (**Scheme**1). The imine group was appeared at 1643 cm^{-1} and 8.01 ppm in IR and 1H NMR spectra respectively.



Scheme1: The structure of a typicality of new Schiff base ligand
X= Different amines with cyclohexane group.

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Synthesis and Characterization of New Schiff Base Ligands with S and N Donor atoms

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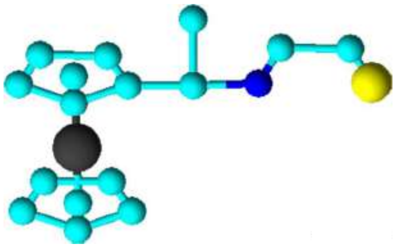
Keywords: Schiff Base, Ligand, Linear Amine, Fluorescence, Spectroscopy

Schiff base ligands are the most important ligands because they are easily synthesized using the condensation reactions between the compounds containing carbonyl groups and primary amines. Schiff base ligands can coordinate with many different transition metals, and form stabilize complexes with different oxidation states [1]. These ligands show a wide range of biological properties such as anticancer, antitumor, antifungal, antibacterial, antimalarial, antiviral and anti-HIV activities. Schiff base complexes have been shown to possess catalytic activity for the polymerization or copolymerization of olefins and vinylic monomers [2]. In this work, new Schiff base ligands were synthesized from the 1:1 and 1:2 molar condensations of diacetyl, acetyl and different aldehydes with linear amine containing N and S donor atoms at 60 °C in ethanol (**Scheme1**). The Schiff base ligands showed photoluminescence in methanol at room temperature. The Schiff base ligands can coordinated to metal ions as a through nitrogen and sulfur donor atoms. The synthesized compounds were characterized by FT-IR, ^{1}H NMR, UV-Vis spectroscopies and elemental analysis. The functional group of imine ligand was appeared in the range of 1603-1665cm^{-1} and 8.00-9.00 ppm in IR and ^{1}H NMR spectra, respectively.



Scheme1: The structure of new Schiff base ligand.

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Design and synthesis of metal-organic framework based on zirconium in the synthesis of tetrahydropyrido[2,3-d]pyrimidines

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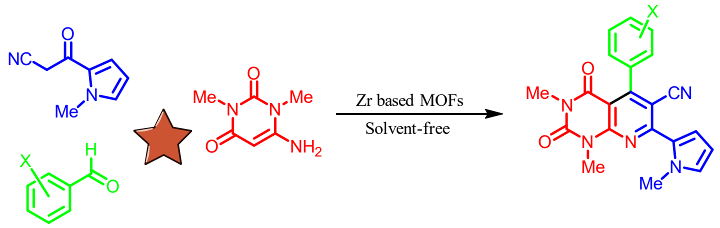
Keywords: Metal Organic Frameworks (MOFs), Zirconium, Tetrahydropyrido[2,3-d]pyrimidines, Catalysts and organic compounds

Metal-organic frameworks (MOFs) have been known as a unique type of porous solid materials, because they have been utilized in different fields such as drug delivery, catalyst, photocatalyst, battery, super capacitor, sensor, gas storage, separation and adsorption of molecules [1]. Among them, the post-modification of metal-organic frameworks can be carried out with metal, acid and basic groups for preparation of biological molecules, which make motivational enzymes attractive for catalytic processes. Thus, post-modification improves the performance of the structure of metal-organic frameworks (MOFs) by applying changes in surface, pore size, thermal and chemical stability [2]. *N*-heterocycle compounds such as tetrahydropyrido[2,3-d]pyrimidine structures are an important class of organic compounds with unique medicinal and biological properties. Also, schaffolds based on pyrole, pyridine and 1,4-dihydropyran moieties have been studied in various pharmaceutical fields as antitumor, painkiller, antihypertensive, anti-inflammatory, antifungal and antimicrobial drugs. In the above work, Zr based MOFs with high surface area and high pore volume was synthesized. The above catalyst was used in the synthesis of tetrahydropyrido[2,3-d]pyrimidine derivatives. The high reaction efficiency, short reaction time, reducing the production of side products and the ability to recycle the catalyst are among the features of the above work (**Scheme1**).



Scheme1: Preparation of tetrahydropyrido[2,3-d]pyrimidines using Zr based MOFs

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Solid phase synthesis of cobalt-tungstate pigment on mica

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Keywords: Cobalt-tungstate, Pigment, Mica

Mineral pigments have been considered important materials for human life for many years. Special effect pigments with the most important types, pearl luster and interference pigments, are based on natural or synthetic materials. They show outstanding qualities of luster, brilliance, and iridescent color effrcts based upon optically thin layers [1]. $CoWO_4$ pigments are widely used in various industries. In this article, it has been tried to explain the formation of pearlescent pigments consisting of cobalt tungstate particles on mica surfaces under optimal conditions. An easy and low-cost method has been used to produce blue mica/$CoWO_4$ pearl pigments. The synthesized samples were characterized by XRD, FESEM-EDX, UV-Vis-NIR diffuse reflectance spectroscopy, and CIE L*a*b* color scales. Composite pigments prepared using 50% $CoWO_4$ and 50% mica have a beautiful effect and light blue color [2]. The synergistic effect of mica and cobalt tungstate on each other has made the total value and performance of mica and $CoWO_4$ pigment greater than their individual value and performance [3]. The results showed that the luster and color characteristics of pearl composite pigments are affected by the size change and the amount of mica used.

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Preparation of electrochemical sensor based on silver nanoparticles for sensitive detection of chloramphenicol

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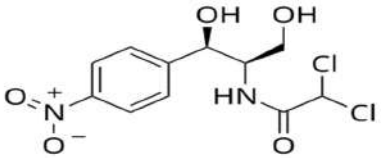
Keywords: Antibiotic, Sensor, Real sample

Chloramphenicol (CAP) with the chemical formula $C_{11}H_{12}Cl_{2}N_{2}O_{5}$ is an antibiotic for the treatment of bacterial infections (**Scheme1**). CAP is a strong antibiotic that is used in the control and treatment of bacterial diseases (tuberculosis and typhoid) in animals and humans, especially against Gram-positive and Gram-negative bacteria. The presence of the nitrogen group attached to the benzene ring in the chemical structure of CAP and being known to be toxic caused its use in sterile eye drops and eye ointment to be minimized. The consequences of excessive use of this antibiotic in milk and contaminated food for pregnant mothers led to the birth of children with diseases such as: irregular breathing, collapse of the vasometer and pale cyanosis. In adults, it leads to aplastic anemia, blood and brain cancer, depression and increased blood pressure. The maximum amount of CAP in food products should be less than 0.3 micrograms per kilogram. Therefore, it is desirable to develop a simple, low-cost, fast and sensitive method to identify antibiotics, especially CAP [1]. Electrochemical methods have many advantages, such as ease of access, low cost, short time, high sensitivity, fast response, measurement of low amounts, high selectivity and reproducibility, which compared to other analytical methods, pay a lot of attention to have attracted themselves [2]. Based on this, we prepared silver nanoparticles by co-precipitation method. After preparing GCE modified with silver nanoparticles using electrochemical techniques such as cyclic voltammetry, the efficiency of the prepared Ag/GCE sensor was checked in the presence of drug in 0.1 M phosphate buffer, pH = 7 and finally in real samples of milk and honey. The obtained results indicated that in the presence of CAP with a concentration of 0.1 mM, a current of 20 µA and a peak of 0.75 V was obtained for GCE, and a higher current of 50 µA and a peak of 0.45 V was registered, which shows the good catalytic activity of this electrode for the detection of chloramphenicol as electrochemical sensor.



Scheme1: Chemical structure of chloramphenicol.

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Application of Organic-Inorganic Hybrid Bionanocomposite from Cellulose and Nanoclay for Cationic Dye Removal

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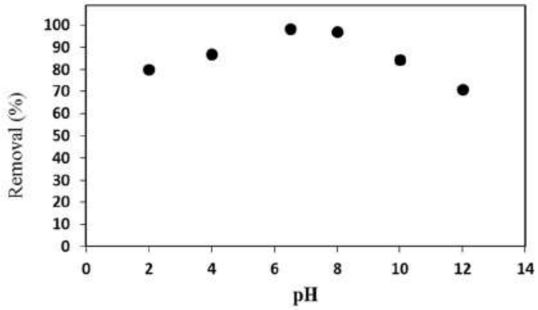
Keywords: Nanoclay, Cellulose, Bionanocomposite, Adsorption, Cationic dye

Clays are inorganic naturally occurring environment-friendly materials possessing high specific surface area and good cation exchange capacity. It is known for its accumulative capacity for water-soluble hazardous and toxic dyes on the surface [1]. The nanoclay composites with biopolymers gained much attention since composites have unique properties and structural diversity, which offers superior performance versus individual counterparts [2]. This paper reports a facile method for the preparation organic-inorganic hybrid bionanocomposite from cellulose and nanoclay for cationic dye, navy blue 2RN removal from aqueous solution by batch adsorption techniques. Bagasse was used as a cellulose source, while nanoclay was obtained from Nanocore Inc., which was modified chemically before composite preparation. The optimal conditions for the dye adsorption were found to be pH = 6.5, initial dye concentration: 40 mg/L and adsorbent dosage of 100 mg. The adsorption efficiency of dye molecules were 98.61% (Scheme 1). The entire adsorption process was completed within 60 min. The cellulose/nanoclay nanocomposite showed remarkable adsorption efficiency for dye removal in wastewater treatment process and could possibly be used for the treatment of textile effluents.



Scheme 1: Effect of pH on removal of cationic dye by cellulose/nanoclay nanocomposite

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Adsorption Removal of Direct Dye from Aqueous Solution using Inorganic Nanoclay and Activated Carbon

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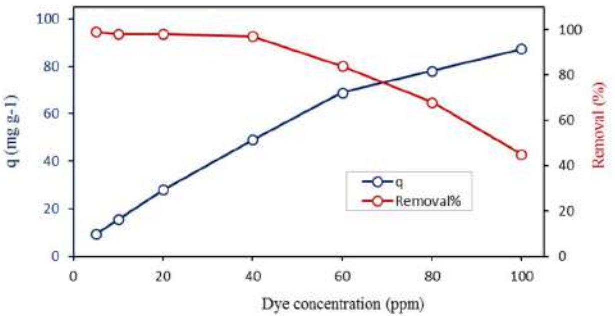
Keywords: Nanoclay, Activated carbon, Adsorption, Direct dye

Wastewater generated from the textile industry is a major contributor to water pollution due to the use of synthetic dyes in textile production. Inorganic nanoclays are suitable adsorbents for textile dyes adsorption among many other commercial adsorbents due to their non-toxicity, abundance and hence availability, high specific surface area and pore volume, low cost, high ion exchange capability and great adsorption characteristic [1]. To increase the adsorption performance of nanoclay, it can be composed with other adsorbents e.g. activated carbon. There is no doubt that the combination of different efficient adsorbent materials would improve their adsorption capacity, featuring with all integrated characteristics inherited from the constituents [2]. In this study, an attempt has been made to remove a direct dye, direct blue 71 using a composite adsorbent which is a combination of nanoclay and activated carbon prepared from apricot seed shell. The effectiveness of the prepared composite to remove direct blue 71was examined at different initial dye concentrations, adsorbent dosage and pH. Results reveal that the equilibrium was attained within 45 min having 0.8 g/L adsorbent at pH of 4 and initial dye concentration of 40 ppm and the maximum equilibrium capacity was observed 87.3 mg/g (Scheme 1). It can be concluded that the nanoclay/activated carbon composite can have a great potential for textile waste water treatment.



Scheme1: Effect of initial dye concentration on dye adsorption capacities and removal efficiencies.

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Efficient bi-Functional catalyst for one-pot tandem oxidation/Knoevenagel condensation reaction

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Keywords: Tandem Reaction, Oxidation, Knoevenagel condensation, Metal-Organic Framework

Tandem reactions, which enable multistep reactions in one pot, have attracted significant interest because they eliminate the need to isolate intermediates and minimize waste production, providing substantial economic benefits [1]. Multifunctional catalysts which contain different catalytically active sites in a site-isolation manner to maintain their independent function are typically essential for efficient one-pot tandem reactions [2]. Significant efforts have been dedicated to designing heterogeneous catalysts for tandem reactions by immobilizing metal complexes and nanoparticles onto the surfaces of various porous supports. Metal-organic frameworks (MOFs) which are constructed from metal ion clusters bridged by multidentate organic linkers, are exclusively exploited in various valuable applications. In this work, bifunctional heterogenous catalysts were constructed by incorporation of different cyanide functional groups into HKUST, characterized by means of XRD, TGA, BET, SEM, FTIR and elemental analysis, and utilized in one-pot tandem oxidation/Knoevenagel condensation reaction for diverse benzyl alcohols. Highly selective catalytic activity was observed for the modified frameworks with 55–100% conversions and 85–100% selectivity toward the desired product. Investigation of the stability and reusability of the catalysts revealed the heterogeneity character of the catalyst with no desorption during the course of oxidation reactions.

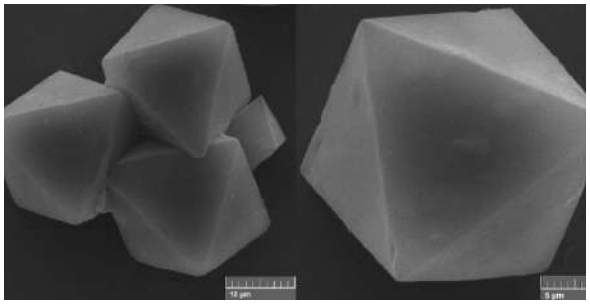

Fig.1. SEM image of the synthesized and modified framework.

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Exploring the Efficacy of Magnetic Covalent Organic Framework Composites in Water Treatment

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Keywords: Magnetic covalent-organic framework, Organic pollutant, Wastewater

Industrial wastewater poses serious environmental challenges due to toxic, carcinogenic, and mutagenic organic pollutants and their by-products, which resist decomposition. These contaminants threaten aquatic life, disrupt plant ecosystems, and pose human health risks [1]. Various processes have been employed to treat effluents with differing efficiencies. scientist is trying to struggle to remove organic pollutants due to their persistent, non-biodegradable nature. Photocatalysis is a proposed method that degrades these pollutants, converting them into inorganic compounds such as water and carbon dioxide [2]. The efficacy of magnetic covalent-organic framework composite in degradation of organic pollutants, from aqueous solutions was investigated. The research exhibited that the process follows first-order kinetics. Also, the composite displayed good stability, maintaining its performance over five cycles [3].

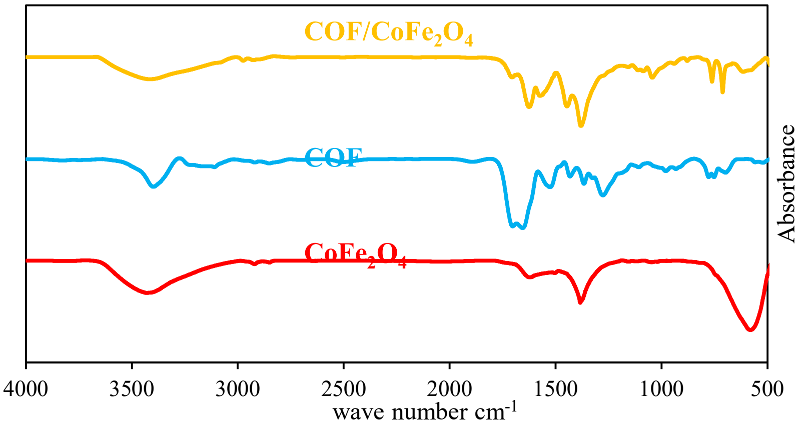

Fig 1. FTIR spectra of samples.

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A Cycloplatinated(II) Complex Bearing a Phosphorus Donor Ligand: Synthesis, Characterization, and Biological Evaluation

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Keywords: Cycloplatinated complexes, Phosphine ligands, Biological activity.

Classical auxiliary ligands, such as phosphines, are widely used in various organometallic and coordination chemistry areas [1]. These ligands support various transition metal complexes due to their unique electronic and steric properties [2]. Herein we describe the preparation and characterization of cyclometalated platinum(II) complex [Pt(*p*-MeC_6H_4)(O-bpy)(PPh_2py)], **1**, O-bpy = 2,2′-bipyridine *N*-oxide, PPh_2py = 2-(diphenylphosphino)pyridine (**Figure 1**). The biological activity of this complex was assessed against a panel of standard cancer cell lines, as well as its properties in comparison to the methyl analogue complex [PtMe(O-bpy)(PPh_2py)], **2**. The results showed that this complex had a significant effect against the tested cancer cell lines.

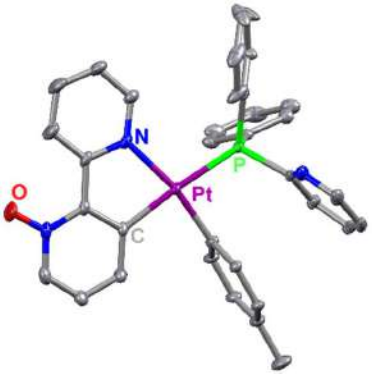

Figure 1. Molecular structure of **1**.

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Synthesis of chitosan-EDTA-β-cyclodextrin polymer for adsorption of Cd(II) and ciprofloxacin micropollutants

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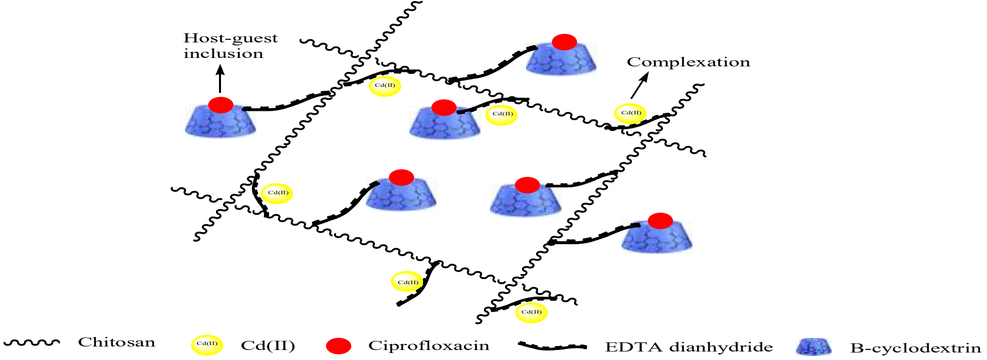
Keywords: Chitosan, β-cyclodextrin, Ciprofloxacin, Cd(II), Adsorption capacity

The current research is about how to synthesize a chitosan-EDTA-β-cyclodextrin (CS-ED-CD) polymeric adsorbent that uses EDTA as a cross-linker to remove cadmium ions and ciprofloxacin micropollutants from wastewater. A possible adsorption mechanism for the removal of Cd(II) and ciprofloxacin pollutants is proposed in (**Scheme1**). The immobilized CD cavities capture the target ciprofloxacin molecules through host-guest inclusion interaction [1], and EDTA groups act as both cross-linkers and adsorption sites for metal ion complexation [2], while chitosan chain is considered as the backbone. The effect of pHs 2, 4, and 6 on the removal of Cd(II) and ciprofloxacin pollutants by CS-ED-CD shows that with increasing pH, the decrease in the surface potential enhanced the electrostatic attraction, resulting in a rise in the removal efficiency. The effect of contact time on the adsorption of each pollutant by CS-ED-CD shows that the removal efficiency increases with increasing time. The ciprofloxacin and Cd(II) removal efficiency received to 87.6 and 89.8%, respectively, over a period of 240 min. The adsorbent displayed adsorption capacity of 43.8, 45.0 mg g^{-1} for ciprofloxacin and Cd(II) respectively.



Scheme1: The schematic illustration of the related adsorption mechanisms of CS-ED-CD toward Cd(II) and ciprofloxacin.

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Construction of Rh(III) Complexes Containing Diphosphinoferrocene Ligands: Electrochemical and DFT Calculations

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Keywords: Rhodium complexes, Ferrocene ligands, Theoretical calculation

Ferrocenyl phosphine compounds represent a prominent group, widely utilized in organometallic and coordination chemistry [1]. Notably, 1,1′-diphosphinoferrocenes (dpf) are significant biphosphine ligands that exhibit multiple coordination modes with various transition metal complexes. These dpf complexes find applications across diverse fields, including catalysis, materials science, electrochemistry, and biology [2, 3]. In this study, we synthesized binuclear complexes by linking two Rh(III) entities using various dpf ligands (**Figure 1**). The complexes were characterized through different spectroscopies, while density functional theory (DFT) was employed for geometry optimization, focusing on the molecular orbital (MO) compositions of occupied and unoccupied fragment orbitals. All calculations were performed using Gaussian software. The B3LYP functional was used in combination with the 6-31G(d) basis set for all elements, except for Rh and Fe, for which the LANL2DZ basis set was used. Also, the electrochemical behavior of these complexes is investigated.

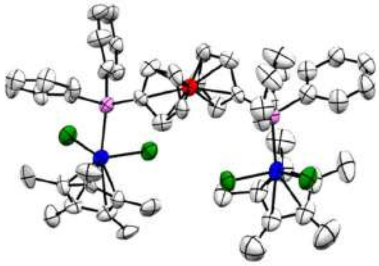

Figure 1. Molecular structure of Rh(III) complex containing a dpf ligand.

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Preparation of Chitosan Hydrogel Containing Phthalocyanine as a Photosensitizer,

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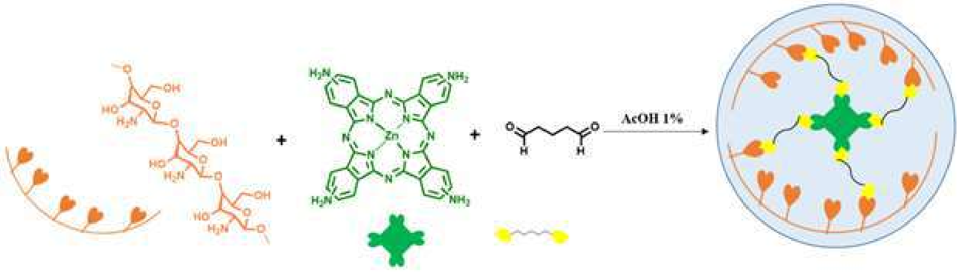
Keywords: Hydrogel, Photosensitizer, Phthalocyanine

Chitosan hydrogel networks have attracted considerations toward their usages in different fields of science ranging from biochemical to biomedical researches [1-2]. Homogeneous chitosan hydrogel networks containing zinc tetraamino-phthalocyanine (ZnTAPc) as photosensitizer prepared though cross-linking with glutaraldehyde. The cross-linking process occurs via imine bond formation by reaction of NH_2 groups of ZnTAPc and chitosan with aldehyde groups of the glutaraldehyde. Insertion of ZnTAPc interestingly increases its solubility in water medium. 2.0% and 4% w/w of the ZnTAPc were used with respect to chitosan polymer to generate hydrogel photosensitizer. FT-IR and UV–Vis spectroscopy, scanning electron microscopy, and rheological measurements were applied to evaluate the properties of the prepared hydrogels (**Scheme1**).



Scheme 1: Preparation of hydrogel containing ZnTAPc cross-linked with glutaraldehyde.

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Hydrogels for Carrying Zinc Phthalocyanine as a Photosensitizer and Difloxacin as an Antibacterial Agent,

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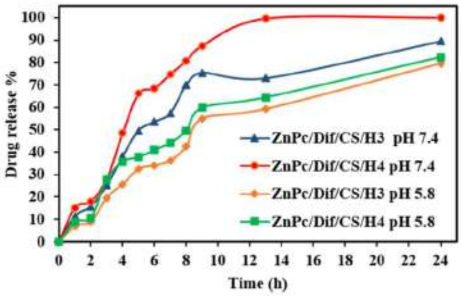
Keywords: Hydrogel, Difloxacin, Antibacterial Agent, Phthalocyanine

Antibacterial resistance has intensified the demand of new drug designs for treatment of bacterial infections. Antibacterial photodynamic therapy (PDT) is an encouraging treatment proposed for various microorganisms. Phthalocyanines have been broadly used as photosensitizers in PDT. However, the application domains of phthalocyanines are restricted by their poor solubility. Fluoroquinolones are synthetic antibiotics known to play an important role in controlling bacterial infections [1-2]. A chitosan hydrogel matrix containing zinc *tetraamino-phthalocyanine* (ZnTAPc) and difloxacin has been designed. It is supposed that the new matrix will show interesting biological activities (**Scheme1**). The results indicated that the difloxacin release rate is faster at pH 7.4 than pH 5.8. The prepared hydrogels generate singlet oxygen under visible light irradiation with good efficiency. So the hydrogels containing both ZnTAPc and difloxacin can be good candidate in chemo-photodynamic therapy.



Hydrogels cross-linked with 1% w/w of glutaraldehyde proportion to the mass of chitosan

Entry	Hydrogel	Chitosan	ZnTAPc	Difloxacin
1	ZnPc/CS/H1	0.15 g	2% w/w	-
2	ZnPc/CS/H2	0.15 g	4% w/w	-
3	ZnPc/Dif/CS/H3	0.15 g	2% w/w	6.67% w/w
4	ZnPc/Dif/CS/H4	0.15 g	4% w/w	6.67% w/w

Scheme1: Drug release from different prepared hydrogels.

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Synthesis and Characterization of New Schiff Base Ligands Containing Ferrocene Group

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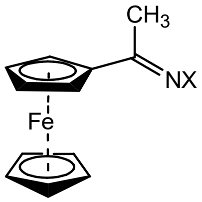
Keywords: Schiff Base, Ligand, Ferrocene, Amine, Acetyl

During the last decades, great attention has been focusedon the area of Schiff bases and their due to the electrontransfer pathways in biological systems [1].Schiff base ligands have been extensively investigated in coordination chemistry due to their facile synthesis, steric, electronic properties, good solubility. Schiff base ligands were coordinated with most of the transition metals easily. Moreover, they show interesting properties like ability to reversibly bind to oxygen, catalytic activity in hydrogenation of olefins and biochemistry [2]. In this work, we reported the synthesis of new Schiff base ligands containing amines with cyclohexane and different derivatives of ferrocene with carbonyl groups. The reactions were performed in 1:1 M ratio of amines and acetylin drymethanolsolution at room temperature and under inert atmosphere for 72hours.
These compounds were characterized by FT-IR, ^{1}HNMR, UV-Vis spectroscopies andelementalanalysis.Thefunctional group of imine ligand was appeared at 1635 cm^{-1} and 8.00 ppm in IR and ^{1}H NMR spectra respectively (**Scheme1**).



Scheme1: The structure of atypicality of new Schiff base ligand
(NX= Different amines containing cyclohexane groups.

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Graphene oxide @ Schiff base of chitosan composite material as adsorbent in removing methylene blue dye from wastewater

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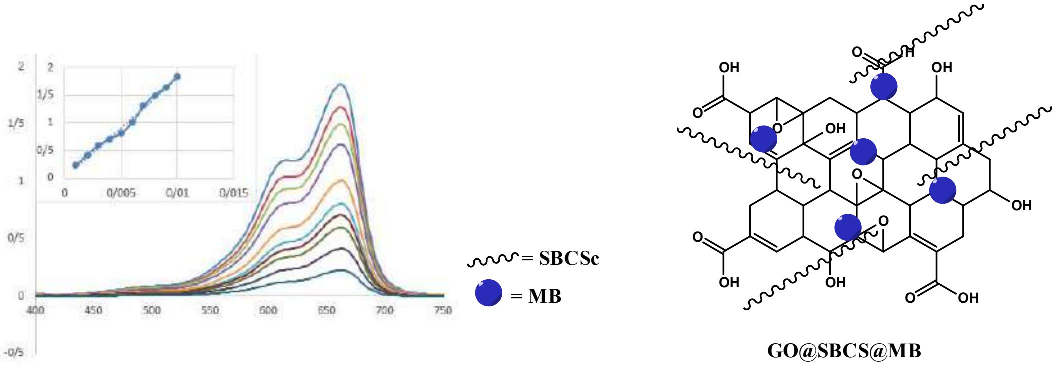
Keywords: Graphene oxide, Schiff base Chitosan, Water Treatment

Water contamination from a wide range of toxic pollutants has posed a great threat to the environment due to their potential human toxicity. Dyes represent one of the problematic groups. Dyes can be classified as follows: anionic/acidic, cationic/basic and non-ionic disperse dyes, and most dyes are aromatic azo type, which can cause health problems such as allergic dermatitis, skin irritation, cancer and mutation in human [1]. Since dye pollution can lead to serious results, it is urgent to search for effective methods to move dye from effluents before they are mixed up with unpolluted natural water bodies. Graphene oxide (GO) has been regarded as promising adsorbent in treating water pollution[2]. However, the high dispersibility of GO makes the separation of adsorbent/pollutant composite from aqueous environment very difficult. In this study, GO was fabricated with Schiff base of chitosan (SBCS) for methylene blue (MB) removal, where GO-SBCS composite was not dispersible in water and could be easily separated by filtration or low speed centrifugation (**Scheme1**).



Scheme1: Schematic absorption of methylene blue by GO@SBCS

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Synthesis and Characterization of NiCoMOF@CF Electrodes with Superior Charge Storage Capabilities

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Keywords: Metal-organic frameworks, Supercapacitors, Solvothermal, Carbon Felt

In this study, we synthesized binder-free NiCoMOF@CF electrodes by a facile solvothermal process. After that, the electrochemical properties of prepared NiCoMOF@CF are characterized by various techniques. The electrochemical investigations of the prepared materials for the Positive electrode were performed in a 3 M KOH electrolyte in a three-electrode cell configuration. The CV of the NiCoMOF@CF electrode under various scan rates is shown in Fig. 1a. The oxidation and reduction peaks in the CV plots of NiCoMOF@CF electrode are observed, but the current density and potential window are diverse, with different scan rates. The pseudocapacitive behavior of the NiCoMOF@CF electrode is confirmed by the redox peaks in the CV plot. As the scan rate increases from 2 to 10 mVs^{-1}, the area of separation of the cathodic and anodic peaks gradually increases exhibiting excellent charge storage behavior of the electrode. As shown in Fig. 1b, the non-linearity of the discharge curves supports the pseudocapacitive nature of the NiCoMOF@CF electrode which is consistent with the findings from CV curves. [1] The maximum areal specific capacity calculated using the discharge curve for the NiCoMOF@CF electrode is found to be 3.04 C cm^{-2} at 4 mA cm^{-2} (Fig. 1c). The Nyquist plot for the NiCoMOF@CF, suggesting rapid charge transfer within the NiCoMOF@CF electrode (Fig. 1d).

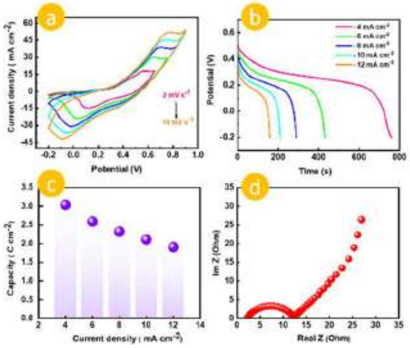

Fig. 1: CV curve of NiCoMOF@CF electrode at various scan rates (a), Discharge curves of NiCoMOF@CF electrode at various current densities (b), Rate capability (c), Nyquist plots of the NiCoMOF@CF electrode at open circuit potential (d).

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Heterogeneous oxidation of alcohols with hydrogen peroxide catalyzed by Polyoxometalate Metal-Organic Framework

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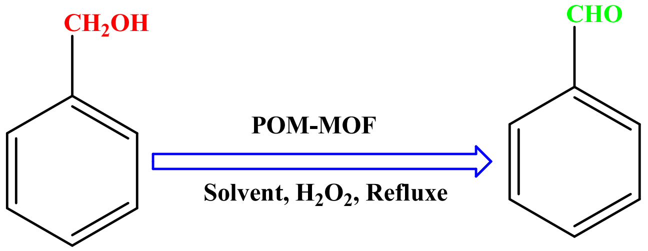
Keywords: Alcohols, Heterogeneous catalysis, MOF polyoxometalates, H_2O_2

HSiW-MOF, PMo-MOF, HPMo-MOFand PW-MOF have been used for selective oxidation of alcohols with hydrogen peroxide. PW-MOF was showed higher catalytic performance compared other catalysts in this reaction condition. PW-MOF is stable, recyclable catalysts for the selective oxidation of a wide range of alcohols to aldehydes, ketones in a acetonitrile with hydrogen peroxide. PW-MOF showed Excellent catalytic activity for selective oxidation of various alcohols in the oxidation reactions. Also, Allylic alcohols were also converted to the corresponding aldehydes with high conversion and selectivity.



Scheme 1: oxidation of alcohols with H_2O_2 catalyzed by POM-MOF.

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Keplerate-type polyoxometalate and Ionic liquid as effective hybrid catalyst for selective epoxidation of different alkenes with H_2O_2

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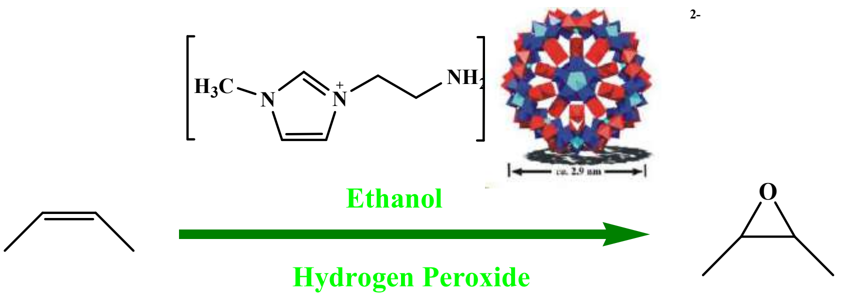
Keywords: Polyoxometalate, Epoxidation of alkenes, Hydrogen peroxide, Ionic liquid

A hybrid catalyst based on Mo132 as a Keplerate type polyoxometalate and MimAm as an ionic liquid was synthesized and approved as an effective catalyst for selective epoxidation of different alkenes with H_2O_2 as a green and safe oxidant. This catalyst complies with the advantages of steady reuse, convenient recovery, simple preparation, high catalytic activity, simplified workup, and flexible composition. The effects of the catalyst and oxidant amounts, reaction time, and temperature were also investigated in detail. Moreover, under the optimal reaction conditions, the epoxidation of different alkenes was achieved with 54-100% yields.



Scheme 1: epoxidation of alkenes with hybrid polyoxometalates

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Lithium extraction by H_2TiO_3 from the salt lake of Qom

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Keywords: Lithium, Brine, Qom salt lake, Adsorbent

Lithium is the third element of the periodic table and the lightest alkaline earth metal in the world with a density of only 0.534 g/cm3at room temperature. causing it to be rarely considered for industrial applications in recent decades with research and innovation in the background of lithium ion batteries and their widespread use in electric vehicles. The brines are one of the most important sources of lithium in nature, and so far, various studies have been conducted in the field of extracting this metal from them [1-3].

In this research a lithium absorbent sample H_2TiO_3 was prepared by the solid phase reaction method from lithium carbonate and titanium oxide as initial compounds. In this synthesis, first we mix and grind the raw materials well then transferred it to a furnace for 4 hours at a temperature of 700 °C. Then it cooled down slowly and reached the ambient temperature, a white Li2TiO3 powder was formed (yeild 88.7%).

The product was stirred with 0.2 M hydrochloric acid for 24 hours, then filtered and washed with deionized water and dried to prepare H_2TiO_3. The compounds were identified by IR and XRD analyses.

In the following, the adsorbent's ability to extract lithium from standard solutions as well as the brine of Qom salt lake was studied. For this purpose, different amounts of adsorbent were used for 12 and 24 hours.

At this stage, the amount of 0.03 grams of the adsorbent was mixed with 10 ml of the sample from the salt lake of Qom, the control sample, the standard solution of lithium carbonate 40 ppm for 8, 12 and 24 hours, then the solution was filtered and then the amount of lithium was measured by Flame Photometer was used. The results showed that increasing the pH to 8, increasing the concentration of the adsorbent and increasing the contact time between the solution and the adsorbent increases the absorption of lithium by the adsorbent.

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Lithium extraction by manganese adsorbent from Qom salt lake

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Keywords: Lithium, Brine, Qom salt lake, Adsorbent

Lithium is a strategic metal and a rare element in the earth's crust, which has many industrial and valuable applications. In addition to minerals, lithium is mainly found in sources such as sea water, salt lakes and geothermal salt water. Research on the development of lithium separation technology from brines is an important and inevitable thing due to its high storage capacity and low cost [1,2].

In this research, using the Sol-gel method with raw materials $MnSO_4$ and Li_2Co_3, a lithium absorbent sample with the formula HMn_2O_4 was prepared with an efficiency of 70.6%.In this synthesis, we put the solution of lithium carbonate in a ratio of 1:4 with manganese sulfate solution on the heater, and while stirring slowly, the solution evaporates and turns into a gel, then We transfer it to a porcelain crucible and place it in an oven at a temperature of 800 degrees Celsius for 5 hours. The obtained product is a vermilion powder of $LiMn_2O_4$.

The resulting material is mixed with 0.2 M hydrochloric acid for 24 hours at a slow speed, then we filter it until the acid is separated, rinse it with deionized water and let it dry. The product was identified with the help of IR and XRD analyses.

In the following, the adsorbent's ability to extract lithium from standard solutions as well as the brine of Qom salt lake was studied. For this purpose, different amounts of adsorbent were used for 12 and 24 hours at two different pH. At this stage the adsorbent was mixed with the certain amount of sample from the salt lake of Qom and the standard solution of lithium carbonate. Finally the solution was filtered and the amount of lithium in solution was measured by Flame Photometer. The results showed that increasing in pH, concentration of the adsorbent and contact time between the solution and the adsorbent increases the absorption of lithium.

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Molecular Docking Study on the Antipruritic Activity of Avena Sativa Polysaccharides against G-Protein Receptor

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Keywords: Antipruritic, Avena Sativa, G-Protein Receptor, Molecular docking

Itching is the most common skin symptom. The most typical response to itching is the scratching reflex. Scratching damages the skin's epidermis, causing moisture loss and increasing dryness on the skin's surface. Antihistamines, pain modulators, opiate receptor antagonists, and antidepressants are mainly used to relieve itching. Although these drugs have an immediate effect, long-term use will produce tolerance and side effects [1]. Oat (*Avena sativa L.*) is distinct among cereals due to its nutritional value and multifunctional characteristics [2]. Previous studies have highlighted various bioactivities of oat polysaccharides, including immune-modulating effects, cholesterol-lowering effects, intestinal microbiota regulatory activity, and excellent digestibility and hypoglycaemic effects. These potential health benefits make oats polysaccharides a valuable component in oats, prompting increased interest and research in both functional food and pharmaceutical industries [3].

This work focused on the molecular docking study to find the antipruritic active components of oat. Bioactive ingredients are docked to the target proteins (Human G-protein receptor), and the best binding modes are analyzed. The results showed that stigmasterol and β-sitosterol had the most negative binding scores (DS) and the highest ability to inhibit the nominated receptors. Avenanthramide ligands, especially AVA-E and AVA-G, also showed high binding scores. These compounds blocked the active site of the receptor and showed good agonistic behavior in the management of pruritus, so their use in the preparation and manufacture of antipruritic drugs is suggested.

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Structural Characterization of Cycloplatinated(II) Complexes Bearing a Pnictogen Ligand

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Keywords: Cyclometalated complex, Platinum, Pnictogen ligands

Pnictogen (Pn)-based donors, particularly triphenylphosphine (PPh_3), are among the most widely used bulky ligands for transition metal complexes and catalysis [1]. However, there has been limited exploration of its analogous species, such as triphenylarsine ($AsPh_3$) [2]. This is what led to our current research, the cycloplatinated(II) complexes [Pt(*p*-MeC_6H_4)(C^N)(SMe_2)], C^N = 2-phenylpyridine (ppy, **A**); 2-(2,4-difluorophenyl)pyridine (dfppy, **B**); were bearing a labile SMe_2 (dimethylsulfide) ligand, and it could easily and smoothly be replaced with a $AsPh_3$ ligand, which led to the formation of Pt(II) complexes [Pt(*p*-MeC_6H_4)(C^N)($AsPh_3$)], C^N = ppy, **1**; dfppy, **2**, in good yields. These complexes were characterized by usual instrumental techniques such as NMR and X-ray (**Figure 1**).

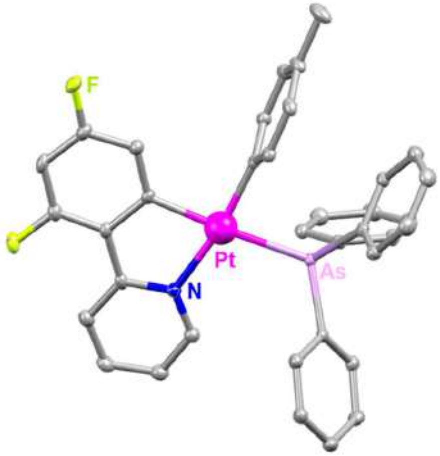

Figure 1. Molecular structure of **2**.

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Kinetic and mechanism of C–I bond activation with fluorinated cycloplatinated(II) complexes bearing phosphine ligands: experimental and theoretical approaches

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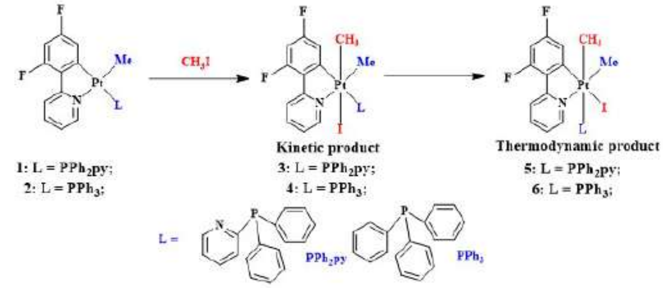
Keywords: Cycloplatinated complexes, Phosphine ligands, Mechanism, Oxidative addition, Kinetic.

Cycloplatinated compounds show distinct kinetics in C-H activation, favoring aromatic products over C-X bonds, influenced by the steric and electronic properties of phosphine ligands.[1] Cyclometalated Pt(II) complexes [PtMe(dfppy)(L)] were synthesized and characterized using HR ESI-mass and NMR techniques as shown in the scheme1. NMR studies of reactions with methyl iodide (MeI) and deuterated methyl iodide (CD_3I) revealed a transformation from trans kinetic products to cis thermodynamic products, with rapid isomerization observed.[2] Kinetic studies indicated a second-order S_N2 mechanism, showing that electronic effects enhance nucleophilic substitution reactivity. DFT simulations provided insights into the reaction mechanism and solvation effects.



Scheme1: Reactions studied in this work.

References

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Investigation of Antipyretic Potential of Lawsonia Inermis L. Phytochemicals Using In-Silico Study

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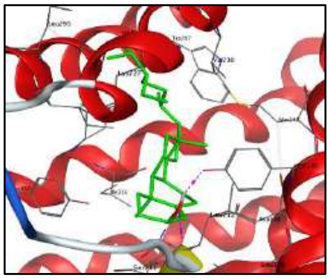
Keywords: Antipyretic, Lawsonia Inermis, Molecular Docking, Phytochemicals

Medicinal plants are important for pharmacological research and drug development when not only plant constituents are used directly as therapeutic agents but also as raw materials for drug synthesis or as models for pharmacologically active compounds [1]. Lawsonia inermis L. (Henna), is regarded as a medicinal plant because has many properties such as antibacterial, antifungal, antitumor antimalarial, hepatoprotective, wound healing, anti-inflammatory, analgesic, antipyretic, memory enhancement, enzyme inhibitor, and antioxidant. Henna has many phytochemical constituents such as carbohydrates, proteins, flavonoids, tannins, phenolic compounds, and fatty acids [2]. An in-vitro study conducted by Humaish showed that the methanolic leaf extract of Lawsonia inermis has a significant antipyretic effect [3].

The present study aimed to evaluate the antipyretic properties of Lawsonia inermis phytochemicals, using an in-silico process. The components of Lawsonia inermis were screened according to Lipinski's rule of five. A molecular docking study was carried out to simulate the interactions between nominated components and the COX-2 protein target (PDB ID: 3LN1), since, the selective inhibition of COX-2 isoenzyme could result in the necessary antipyretic effects [4]. According to the results, Lawsaritol, β-sitosterol, Betulin, Stigmasterol, and Betulinic acid showed the best docking scores, ranging from of -8.27 to -6.94 kcal/mol. These compounds revealed antipyretic activity and can be considered an effective frame for designing new drugs. However, further biological and clinical research is required to ensure their efficacy.


Docking interactions of protein target, 3LN1, with Lawsaritol.

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Synthesis, characterization, and study of DNA interaction of Zn(II) complexes with diamine ligand as potential antioxidants

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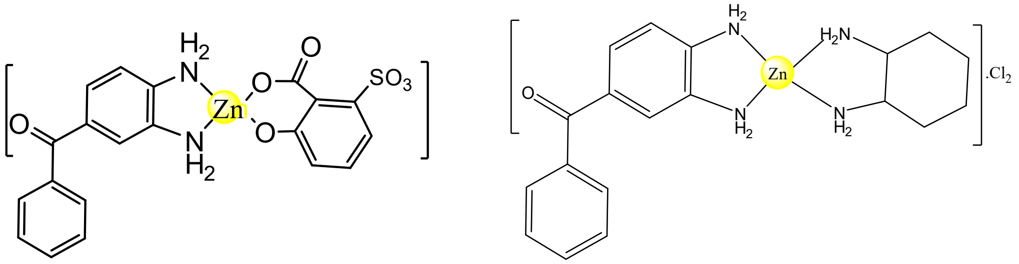
Keywords: Zn(II) complex, DNA-binding, antioxidant activity, electrochemical, Fluorescence properties.

The complexes of [Zn(DAP)(SSA)] (**1**) and [Zn(DAP)(dach)].Cl_2 (**2**) (where DAP is 3,4-diaminobenzophenone, SSA is a dianion of solfosalicylate, and dach is 1,2-diaminocyclohexane) were synthesized (**Scheme 1**) and characterized using various techniques. The interaction of these complexes with CT-DNA was investigated by UV-Vis absorption, fluorescence, gel electrophoresis, cyclic voltammetry (CV), and viscometry. The UV-Vis spectra showed a bathochromic shift of the absorption band and significant hypochromicity at 260 nm for the absorption band of these complexes. The studies show that the interaction of these complexes (**1**, **2**) with CT-DNA occure in two ways; intercalative interaction and groove binding mode [1]. The results obtained from viscosity and electrochemical measurements confirm this. The fluorescence studies showed that the proposed mechanism of fluorescence quenching for both complexes is static quenching. The thermodynamic parameters (ΔH° and ΔS°) revealed that the interaction of complexes (**1**) and (**2**) with DNA is hydrogen bonding and van der Waals. The antioxidant activity of these complexes was investigated with a DPPH (2,2-diphenyl-1-picrylhydrazyl) assay. According to these tests, the antioxidant activity of these complexes compared to vitamin C as a standard antioxidant showed that these complexes are moderate antioxidants [2].



(1) **(2)**

Scheme 1: The proposed structures of new Zn(II) complexes (**1**, **2**).

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In-detailed investigation of DNA/BSA interaction with a dinuclear Zn(II) complex as potential antioxidant by spectroscopic approach

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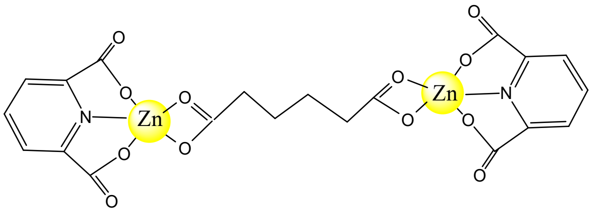
Keywords: Zn(II) complex, Dipicolinic acid, DNA-binding, Antioxidant activity, Electrochemical

A novel complex of $Na_2[Zn_2(dipic)_2\mu\text{-}(Adpic)]$ (**1**) (where dipic is picolinic acid, and Adpic is 1,4-Butanedicarboxylic acid) was synthesized (**Scheme** 1) and characterized using various techniques (FT-IR, ^{1}H-NMR, UV-Vis, elemental analysis, and conductivity measurements). The interaction of this complex with CT-DNA and bovine serum albumin (BSA) was studied by UV-Vis absorption, fluorescence, gel electrophoresis, cyclic voltammetry (CV), and viscometry at blood pH. The results of all these approaches were consistent with a good interaction of the metal complexes with both DNA grooves and BSA via H-binding and van der Waals forces, and electrostatic attraction [1]. The antioxidant activity of this complex was investigated using a DPPH (2,2-diphenyl-1-picrylhydrazyl) assay. The results obtained show that the antioxidant activity of the complex (**1**) compared to vitamin C (as a standard) indicates that it is a moderate antioxidant [2].



Scheme 1: The proposed structure of new Zn(II) complex (1).

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Carbon inks in conductive carbon electrodes of perovskite solar cells

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Keywords: Carbon electrodes, Carbon inks, Solar cells

Integrating carbon inks into perovskite solar cells (PSCs) presents a transformative approach to enhancing the economic and functional viability of solar energy technology. Carbon materials offer a compelling alternative to traditional metal electrodes, which are often costly and require complex fabrication processes. Carbon inks are advantageous due to their low cost, flexibility, and ease of application through scalable printing techniques such as inkjet and roll-to-roll printing, which facilitate large-scale production. These inks enable the fabrication of PSCs under ambient conditions, eliminating the need for vacuum processes and high temperatures, thus reducing energy consumption and manufacturing costs.

Moreover, carbon electrodes exhibit high electrochemical stability and hydrophobicity, improving device stability and longevity. The hydrophobic nature of carbon materials protects the perovskite layer from moisture, enhancing the air stability of PSCs without the need for encapsulation. This characteristic is particularly beneficial for the development of flexible and wearable solar technologies, which require durable and stable materials.

Recent advancements have demonstrated the potential of carbon inks in achieving competitive power conversion efficiencies. By optimizing ink formulations and deposition techniques, researchers have achieved efficiencies that rival those of traditional PSCs, paving the way for commercial applications. The use of carbon inks also aligns with sustainable manufacturing practices, as they are derived from abundant and environmentally benign resources. [1-4]

In this research work, to increase the stability of perovskite against water, a protective carbon ink layer of a mixture of graphite, carbon black, and liquid binder was designed as the electrode. Sheet-resistant analysis, XRD and FE-SEM analyses were used to characterize the layers. Then the performance of the resulting structures in the perovskite solar cell was investigated.

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Synthesis and characterization of copper (II) phen-dione complex supported on nano hercynite as a nanocatalyst for synthesis of organic compound

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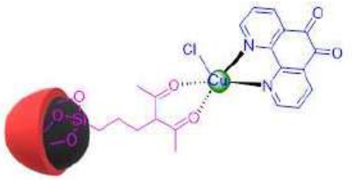
Keywords: Cu(II) complex, 1,10-Phenanthroline-5,6-dione, Hercynite magnetic nanoparticles

One of the key challenges in modern chemistry is the creation of new, efficient catalysts that adhere to the principles of green chemistry. An ideal catalyst should possess several qualities: high activity, selectivity, stability, and low production costs [1]. The coordination environment of a metal complex significantly influences both the energy barrier and the reaction pathway of catalytic reactions [2].

In present work, A novel Cu(II) complex containing 1,10-Phenanthroline-5,6-dione (phen-dione) and Acetylacetone (acac) was innovatively designed and synthesized, and its attachment to silica-modified hercynite magnetic nanoparticles (MNPs) was achieved (**Scheme1**). The resulting structure underwent thorough structural analyses using diverse instrumental techniques. The catalytic potential of the synthesized Cu(II) complex was successfully demonstrated in the synthesis of 2-amino-3-cyano-4H-chromenes. This was accomplished via a one-pot three-component condensation reaction involving lawsone, malononitrile, and aromatic aldehydes in ethanol under reflux conditions, leading to remarkably high yields and product purity. Several advantages stem from this investigation. Notably, the use of ethanol as a sustainable and environmentally friendly solvent highlights the eco-conscious approach of this research [3-5].



Scheme1: [(Hercynite@SiO$_2$@sil-acac)-Cu(phen-dione)Cl] complex.

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Synthesis, characterization and structural analysis of hetero-metallic [Cu_2(μ-L)$_2$Cd(NO_3)$_2$] complex derived from a Salen-type ligand

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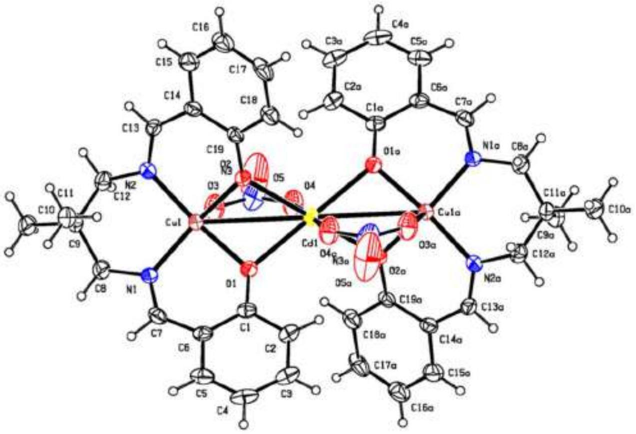
Keywords: Hetero-metallic, ligand complex, Salen ligand

The new trinuclear hetero-metallic copper(II)-cadmium(II) complex, [Cu_2(μ-L)$_2$Cd(NO_3)$_2$], has been synthesized using [CuL] as a so-called ‘‘ligand complex’’ (where L^{2-} = N,N'-bis(salicylidene)-2,2-dimethylpropylenediaminato) and structurally characterized. Compound [Cu_2(μ-L)$_2$Cd(NO_3)$_2$] is a linear hetero-trinuclear complex with a central Cd^{II} ion and lies on inversion centre. This central Cd^{II} ion has an irregular octahedral coordination. The coordination around the Cd^{II} involves four O atoms from two N,N'-bis(salicylidene)]-2,2-dimethylpropylenediaminato(L^{2-}) and two nitrate ligands. The two terminal Cu^{II} ions have an irregular square pyramidal coordination (**Scheme1**).



Scheme1: ORTEPdiagram the complex [Cu_2(μ-L)$_2$Cd(NO_3)$_2$] showing the atom labeling.

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Green synthesis of iron oxide nanoparticles and activated carbon using *Crataegus elbursensis* extract

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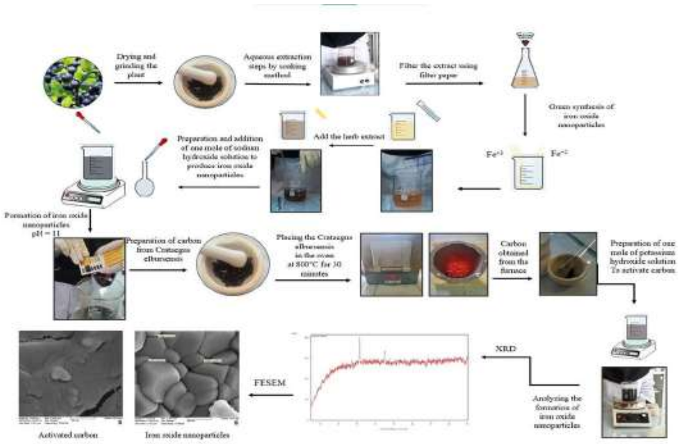
Keywords: Green synthesis, Iron oxide nanoparticles, Activated carbon, Crataegus elbursensis

Recent research has focused on the green synthesis of iron oxide nanoparticles and activated carbon using Crataegus elbursensis extract, attracting attention due to its environmental compatibility and economic benefits. First, C. elbursensis extract was prepared by maceration method and synthesized by green method with 1 M NaOH solution. The carbon prepared from C. elbursensis was activated using a 1 M solution of KOH. XRD and FESEM analysis were used to investigate the morphological properties of nanoparticles. The spectrum obtained from the brush X-ray spectrum (XRD) confirms the purity of iron oxide nanoparticles. The homogeneous spherical nature can be observed using field emission scanning electron microscopy (FESEM) images. Green synthesis is an efficient and effective method for the synthesis of iron oxide nanoparticles, and the activated carbon prepared from C. elbursensis has good porous properties. It can be widely used in industrial fields **(Scheme1)**.



Scheme 1: Graphical abstract of the green synthesis process of iron oxide nanoparticles and activated carbon using Crataegus elbursensis extract

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Fabrication of new solid phase microextraction based on organic-inorganic nanocomposite for determination of organophosphorus pesticides in environmental samples

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Keywords: Nanocomposite, Solid phase microextraction, Organophosphorus pesticides

The use of nanocomposites has been widely spread in the coating of solid-phase microextraction fibers [1]. Chitosan is a natural cationized polymer that is produced from the deacetylation of chitin. In recent years, chitosan-based hybrid materials have been developed due to the excellent properties of individual components and their outstanding synergistic effects [2].

In this project, first, the synthesis of zinc oxide/ silver nanoplates is formed collected, and washed, then its nanocomposite is formed with chitosan. The successful formation of nanoplates (ZnO/Ag) was confirmed by scanning electron microscopy (SEM) and X-ray diffraction (XRD) instruments. Zinc oxide/silver nanoplates and chitosan as a solid phase microextraction fiber coating are used for the extraction and determination of organophosphorus pesticides (diazinon, chlorpyrifos) in environmental samples as a novel and efficient method that was identified by high-performance liquid chromatography (HPLC). The parameters including extraction time, pH, salt percentage, and desorption time were optimized by the central composite design method at 2 min, 8, 20% w/v, and 8 min, respectively. The analytes were desorbed by recovering them in acetonitrile solvent and subsequently injected into a liquid chromatography machine for analysis. The linear range for diazinon was calculated to be 250-900 µg/L, with a qualitative detection limit of 83 µg/L. For chlorpyrifos, the linear range was determined to be 100-700 µg/L, with a qualitative detection limit of 30 µg/L.

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Determination of breast cancer biomarkers with new stir bar with organic-inorganic sorptive extraction

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Keywords: Biomarker, Breast cancer, Stir bar sorptive extraction

The urine is a suitable sample for a volatile metabolomic profiling approach due to the presence of concentrated volatile compounds in this biological fluid [1,2]. Metabolomics of urine have been used to diagnosis of lung, breast, colorectal, prostate and liver cancer [3].

The Poly acrylic acid/MIL-88(Fe)-NH_2 composite material, carefully prepared, is employed as a sorbent for the stir bar. The best formula of the composite was selected by investigation of two parameters including the cross-linker of PAA and MIL-88(Fe)-NH_2 content. The prepared stir bar was used for extraction of 2-pentanone, 2- heptanone, ethyl propionate, para-xylene, 1,2,4-trimethylbenzene, o-cresol, m-cresol in urine samples as breast cancer biomarkers with gas chromatography-flame ionization detector. The prepared Poly acrylic acid / MIL-88 (Fe)-NH_2 as sorbent for the stir bar demonstrate good repeatability of one bar (relative standard deviation (RSD %) < 4.61 %) and satisfactory reproducibility between two bars (RSD% < 6.85 %). The central composite design method was applied for the optimization of extraction parameters. Under the optimum conditions, linear dynamic ranges for compounds were in the acceptable range with correlation coefficients higher than 0.99. Detection limits of them were less than 1.71 $\mu g\ L^{-1}$.

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Palladium complex of 1-(1H-benzo[d]imidazol-2-yl)guanidine on SBA-15@guanidine@Pd(II) as a new, recyclable and efficient nanocatalyst for Suzuki coupling reaction

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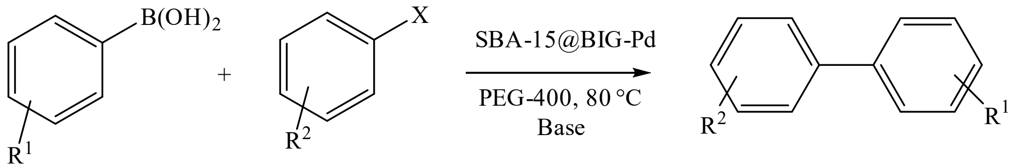
Keywords: Fe_3O_4 magnetic nanoparticles, Schiff-base complex, Heterogeneous catalysts, Zirconium oxide, Copper, Amide

In this work, SBA-15 was synthesized and further modified by (3-Iodopropyl)trimethoxysilane. Then the its surface was functionalized by 1-(1H-benzo[d]imidazol-2-yl)guanidine. Finally, palladium was immobilized on the surface of modified SBA-15 (SBA-15@BIG-Pd). In the second part, SBA-15@BIG-Pd catalyst was identified using ICP, XRD, TGA, BET, FT-IR, SEM, WDX, and EDS techniques. In the final part, SBA-15@BIG-Pd was used as a new, recoverable and practical nanocatalyst for Suzuki coupling reaction through the coupling of aryl halides with phenylboronic acid in PEG-400 as green solvent (Scheme 1). All products were synthesized with high TON, TOF and excellent yield (91-98%) in short times (0.3-3 h), which shows the high efficiency of SBA-15@BIG-Pd. This catalyst can be reused five times without significant loss in its catalytic activity.



Scheme 1: Suzuki coupling reaction in the presence of M-MPAMP@Fe_3O_4 (M=ZrO or Cu).

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Fabrication, crystal structure and antibacterial activity of a novel Cu(II)-Schiff base complex

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Keywords: $CuLCl_2$, Schiff base, Antibacterial activity, Staphylococcus aureus, Escherichia coli

A novel $CuLCl_2$ complex (L = N-(3,4-dimethylphenyl)-pyridine-2-ylmethyleneamine) has been synthesized by two methods. The first method involved the preparation of a single crystal to determine the structure of the complex and $CuLCl_2$ nanoparticles were prepared by the second method. Single crystal X-ray diffraction, NMR, FT-IR, UV–Vis and elemental analysis have been used to characterize the single crystal of the complex (1) and XRD, scanning electron microscopy (SEM), transmission electron microscopy (TEM) and the corresponding particle size distribution histogram has been used to confirm the structure of $CuLCl_2$ nanoparticles (NPs). (**Fig. 1**).

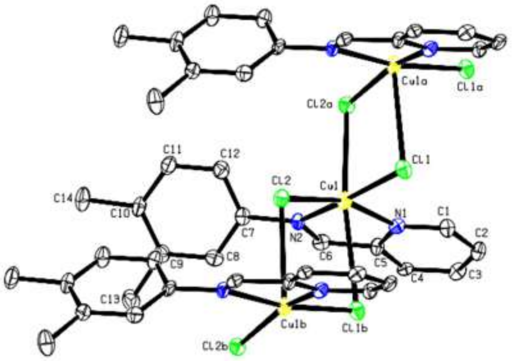

Fig. 1: Crystal structure of complex 1

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Magnetic UiO-66-NH_2 core-shell nanohybrid as a stable heterogeneous catalyst for the preparation of the polyhydroquinoline derivatives

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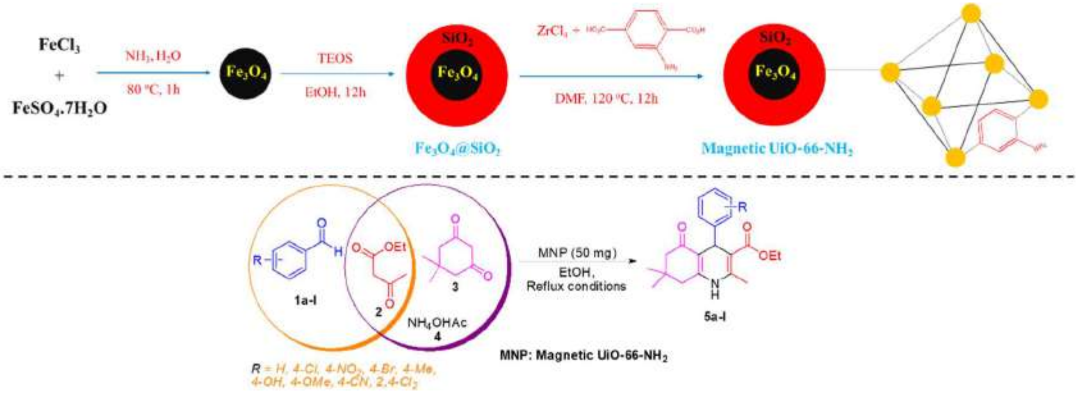
Keywords: Metal-organic framework, Heterogeneous catalyst, Magnetic UiO-66-NH_2

The increasing concerns about the environmental impacts of chemical processes, toxic effects, and energy consumption have underscored the importance of discovering green and sustainable methods for developing materials and compounds. Heterogeneous catalytic systems relying on magnetic nanoparticles (MNPs) are extensively employed in this context because they can be separated through the use of an external magnet. Accordingly, magnetic UiO-66-NH_2 has been synthesized via Fe_3O_4 modification with tetraethyl orthosilicate and subsequently with $ZrCl_4$ and 2-aminoterephthalic acid. A variety of characterization analyses including fourier transform infrared (FT-IR), X-ray diffraction (XRD), fieldemission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), vibrating-sample magnetometry (VSM) and energydispersive X-ray spectrometry (EDX) 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 high efficiency, short reaction time, ecofriendly properties, and easy workup can be considered the major benefits of the current method (**Scheme1**).



Scheme1: Synthesis of magnetic UiO-66-NH_2 and the one-pot synthesis of polyhydroquinoline derivatives.

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Synthesis, characterization, and crystal structure determination of new copper(II) complex $[Cu(L^{pz\text{-}2\text{-}OMe})_2(\eta^2\text{-}NO_3)_2(MeOH)_2]$ with the N-(2-methoxyphenyl)pyrazine-2-carboxamide ligand

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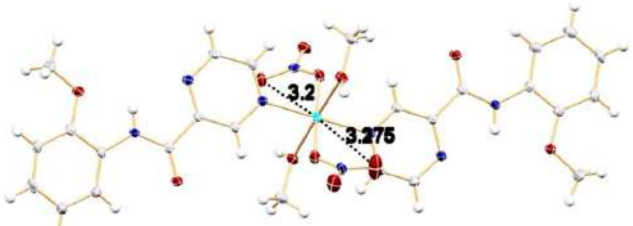
Keywords: Cu(II) complex, Crystal structure, Carboxamide, Pyrazine

Transition metal complexes have attracted enormous attention over the past few decades in materials science, especially for their applications as functional materials [1]. Despite all transition metals, copper has gained much attention due to its enormous biological potential [2–3]. In the present work, the new Cu(II) complex has been designed and synthesized from the reaction of $Cu(NO_3)_2.3H_2O$ with two equivalents N-(2-methoxyphenyl)pyrazine-2-Carboxamide Ligand ($L^{pz\text{-}2\text{-}OMe}$). The crystal and molecular structure of the coordination complex $[Cu(L^{pz\text{-}2\text{-}OMe})_2(\eta^2\text{-}NO_3)_2(MeOH)_2]$ (**Scheme1**), has been determined by X-ray crystallography, IR, and UV-Vis.



Scheme1: ORTEP diagram of the synthesized complex.

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Magnetic UiO-66-NH$_2$ core-shell nanohybrid as a heterogeneous catalyst for the Knoevenagel condensation

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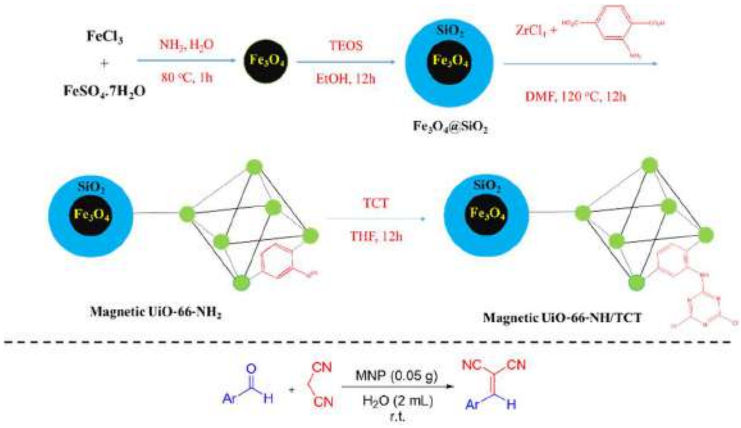
Keywords: Magnetic UiO-66-NH$_2$/TCT, Metal-organic framework, Knoevenagel condensation

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. In the present work, based on a protocol, we synthesized Fe_3O_4@SiO_2@UiO-66-NH$_2$/TCT as a green and recyclable nanocatalyst by an inexpensive and simple procedure. The physiochemical properties of the nanocatalyst prepared were investigated by using Fourier transform infrared (FT-IR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), vibrating-sample magneto-metry (VSM) and energy dispersive X-ray spectrometry (EDX) analyses. The catalytic movement of the synthesized nanocatalyst underwent successful investigation in the Knoevenagel condensation through malononitrile as well as various aldehydes in H_2O 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 (**Scheme1**).



Scheme1: Preparation of magnetic UiO-66-NH$_2$/TCT and Knoevenagel condensation.

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Enhancing Photoelectrochemical Water Splitting Performance with Sorbitan-Modified $CsPbBr_3$ Perovskite Electrodes

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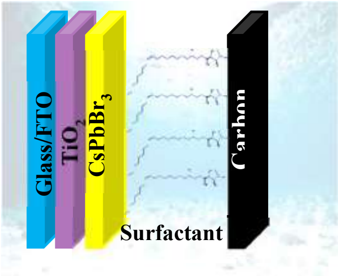
Keywords: Inorganic Perovskite, Surfactants, Photoelectrochemical Water Splitting

Recent studies emphasize the importance of interface engineering in perovskite solar cells and photoanodes for efficient energy conversion [1]. The study investigates the photoelectrochemical (PEC) performance of a $CsPbBr_3$ perovskite electrode modified with a sorbitan monooleate layer, aiming to enhance water splitting efficiency for hydrogen production. Initial experiments with a carbon-coated $CsPbBr_3$ electrode achieved a current density of approximately 3 mA/cm². Subsequent application of a sorbitan monooleate layer followed by carbon deposition resulted in a significant increase in current density to around 4 mA/cm².

This enhancement is attributed to improved charge transfer and reduced recombination losses at the perovskite/carbon interface, facilitated by the sorbitan monooleate layer. The findings underscore the potential of utilizing surfactants to optimize electrode performance in PEC applications, particularly for sustainable hydrogen production [2,3].

This research contributes to the ongoing efforts in optimizing perovskite-based systems for energy applications, highlighting the role of interface engineering in enhancing overall device performance.



Scheme1: The schematic of TiO_2/$CsPbBr_3$/surfactant/Carbon Electrode

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Synthesis and investigation of electrochemical performance of polymer-based ZiF-67/spinel nanocomposite

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Keywords: Supercapacitor, Nanocomposite, Electrochemistry, ZiF-67, $CuCo_2S_4$

In this study, considering the high efficiency of supercapacitors and their widespread applications in various fields such as energy storage and management in modern life, we aim to synthesize and utilize a tri-component nanocomposite based on polymeric $CuCo_2S_4$ and ZIF-67 in supercapacitors to measure and enhance their capacitance and related properties. Binary metal sulfides MCo_2S_4 (M = nickel, zinc, copper, manganese, etc.) have received increasing interest due to their low cost and low toxicity. Among the transition metal sulfides, the binary sulfide ($CuCo_2S_4$) has attracted special attention due to its octahedral Co sites and tetrahedral Cu sites, which offer rich redox states, high theoretical capacity, and environmental compatibility. Polymers are efficient and versatile materials due to their stability and simple synthesis methods. Thus, polymer-based composite materials have been used to construct energy storage and conversion devices. Additionally, zeolitic imidazolate frameworks (ZIFs) belong to a subset of metal-organic frameworks (MOFs) characterized by high surface area, tunable properties, and good chemical stability. These materials are also widely used as precursors for forming composite supercapacitor electrodes. Given all these points, the construction of nanocomposite structures to design supercapacitors with high energy density and stability is essential and represents a significant research challenge.

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Electrochemical detection of chlorogenic acid in green coffee beans by carbon paste electrode modified with MWCNTs and Cr-MOF

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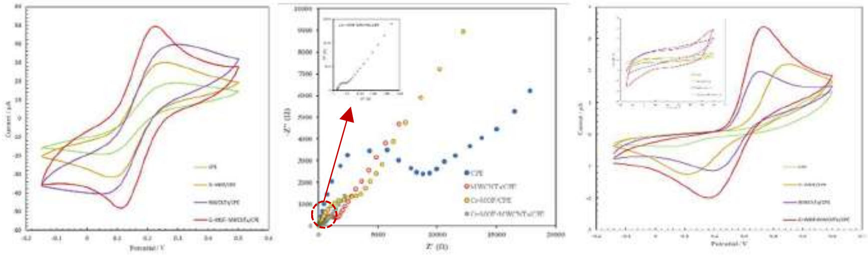
Keywords: Chlorogenic acid, electrochemical sensor, MIL101(Cr), electrochemical detection

Chlorogenic acid is found in many products, including coffee and green tea, and hundreds of medicinal plants[1].In this work, an efficient electrochemical sensor was prepared by combining Cr-MOF and MWCNT with an optimal ratio as a modifier in the carbon paste (CP) electrode. The structure of Cr-MOF and MWCNTs compounds was determined by SEM, EDX, FT-IR and XRD techniques. CV and EIS techniques were also used to investigate the electrochemical performance of the modified electrode. Under optimal conditions, DPV voltammogram showed that the CGA current was in two regions with a coefficient of determination of 0.9855 in the concentration range of 0 to 14.4 µM and a coefficient of determination of 0.9956 in the linear range of 14.6 to 177 µM. Also, the limit of detection (LOD) value was 0.0198 µM, which is very close and competitive with the detection limit of chlorogenic acid measurement with other electrodes[2] . This method has excellent repeatability with a relative standard deviation of 1.39% and high repeatability with a relative standard deviation of 1.25%. In order to measure the CGA present in several samples of green coffee beans, the concentration of CGA obtained by the standard uv-vis method was compared with the concentration obtained by the electrochemical method, and the difference between them was between 1 and 4%. Therefore, a sensitive and reliable sensor for CGA measurement was designed in this work.



Scheme1: (a) CV voltammogram of different electrodes in 5.0 mM K3[Fe(CN)$_6$]$^{3-/4}$. (b). Nyquist diagram. (c). CV voltammogram of electrodes in 0.5 mM CGA. Inset: CV voltammograms in buffer solution (pH=7.0).

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One-Pot, Two-Step Green Synthesis of Ortho-Ortho Ethylenediamine-*N,N′*-Bis(o-Hydroxyphenyl) Acetic Acid/Fe(III) Chelate as a Ferric Fertilizer

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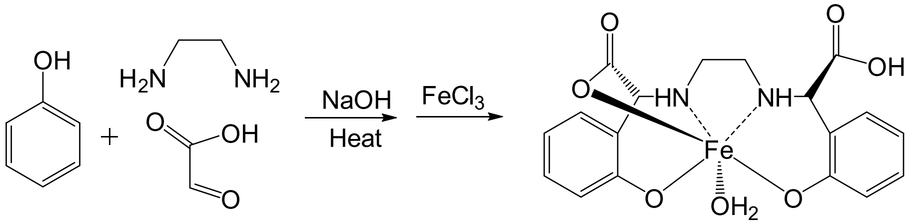
Keywords: Ethylenediamine chelate, Plant nutrient availability, Ferric fertilizer

This study presents an one-pot, two-step green synthesis of ortho-ortho ethylenediamine-N,N'-bis(o-hydroxyphenyl) acetic acid/Fe(III) chelate, aimed at developing an effective ferric fertilizer. Utilizing eco-friendly methodologies, the synthesis employs phenol, ethylenediamine and glyoxylic acid as substrates all dissolved in water to synthesis ortho-ortho ethylenediamine-*N,N′*-bis(o-hydroxyphenyl) acetic acid at 70 °C (**Scheme 1**) [1]. The reaction conditions were optimized to enhance yield and minimize environmental impact. Characterization of the synthesized chelate was conducted using spectroscopic techniques, confirming its structural integrity and chelation efficiency [2]. The resulting ferric fertilizer demonstrated potential for improving nutrient availability and promoting plant growth. This green approach not only reduces harmful waste but also offers a sustainable alternative for agricultural applications [3].



Scheme 1: Proposed structure of ortho-ortho ethylenediamine-*N,N’*-bis(o-hydroxyphenyl) acetic acid/Fe(III) chelate.

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Green synthesis of L-Methionine-Zn(II) complex and its application as animal feed additive

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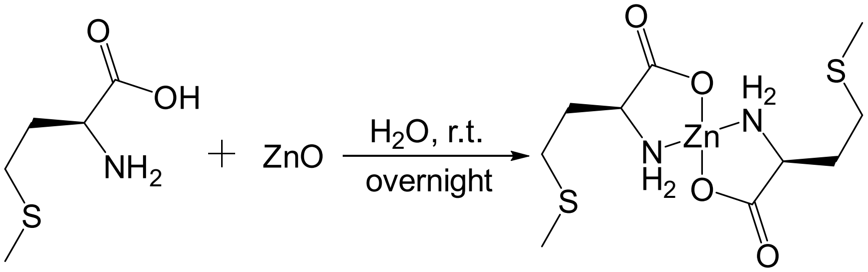
Keywords: Zn(II) complex, Methionine, Amino acid, Animal feed additive, Green synthesis.

This study presents the green synthesis of an L-Methionine-Zn(II) complex using an environmentally friendly approach, without the use of harmful solvents or reagents. The complex was characterized through various spectroscopic techniques, including UV-Vis, FT-IR, and Elemental analysis (CHN), confirming the successful coordination between L-Methionine and Zn(II) [1]. The synthesized complex was evaluated for its potential as an animal feed additive, particularly focusing on its bioavailability and nutritional benefits. Results indicated enhanced zinc absorption and improved overall health markers in animals, demonstrating its efficacy as a sustainable and nutritious alternative to conventional feed supplements. This green synthesis method offers a promising route for producing bioactive complexes in animal nutrition with minimal environmental impact (**Scheme 1**).



Scheme 1: Synthesis of L-Methionine-Zn(II) complex in water.

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Computational Study of Novel Carbenes with Electron-Donating Heteroatoms: Singlet State Stabilization

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Keywords: Carbene, DFT, Electron-donating heteroatoms, Singlet state stabilization, Catalysis

Carbenes, reactive species with a neutral carbon atom and two non-bonding electrons, are widely used in catalysis due to their unique electronic properties [1]. This study presents new carbene derivatives with electron-donating heteroatoms (NH, OH, PH) at position 11, potentially stabilizing the singlet state and affecting reactivity [2]. DFT calculations using the Gaussian 03 software [3] with the B3LYP/6-31+G* method was employed to assess the stability of singlet and triplet carbenes with these heteroatoms.

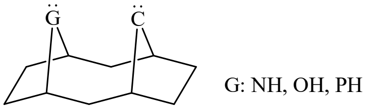

Figure 1: Schematic structure of novel carbene derivatives with an electron-donating heteroatom at position 11 and a carbene carbon at position 12.

Results demonstrated that electron-donating heteroatoms significantly stabilize singlet carbenes in the order NH > OH > PH, attributed to their electron-donating strength and interaction with the carbene center. No significant effect was found for triplet carbenes. The substantial energy gap between singlet and triplet states implies enhanced kinetic stability, which could be beneficial in catalytic applications [2]. In summary, carbene derivatives with electron-donating heteroatoms at position 11 exhibit increased singlet stability through electronic interactions at position 12, showing promise as ligands in organometallic catalysts with tunable electronic properties and reactivity [1, 3].

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Synthesis, characterization, and structure of pyrazine carboxylic acid-based carboxamide ligands and their complexes with copper (II), nickel (II), and cobalt (II) and the ligands application as fluorescence sensor

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Keywords: Carboxamide ligands, Pyrazine, Ionic liquid, Fluorescence sensor, Copper complex, Nickel complex, Cobalt complex

In this project, pyrazine-based carboxamide ligands were synthesized. Carboxamide ligands are particularly important due to the presence of an amide group and have various applications such as catalyst, antibacterial, antitumor, and sensor. The synthesized pyrazine-based ligands and pyrazine compounds have many industrial and biological applications such as disinfectants, insecticides, etc. Unlike the synthesis methods with toxic and dangerous solvents that have been used in the past, these ligands have been synthesized and prepared by the molten salt method, which is a more favorable method. One of the synthesized ligands is N,N'-(1,2-phenylene)bis(5-methylpyrazine-2-carboxamide) (bpzbMe$_2$), which is a novel ligand and its complexes using copper (II), nickel (II) and cobalt (II) metal salts were synthesized. ATR, CHNS, NMR, and UV-Vis methods were used to identify and determine the structure of the ligand and its complexes. Suitable crystals were prepared from bpzbMe$_2$ ligand, and copper and nickel complexes and were analyzed by X-ray diffraction crystallography. In the second part of the project, both ligands bpzbMe$_2$ and N,N'-(1,2-phenylene)bis(pyrazine-2- carboxamide) (bpzbH$_2$) were investigated by absorption and emission spectroscopy. Their behavior in the presence of different metal ions was analyzed, and the results showed that both of them can be used as ON- OFF fluorescence sensors to identify Fe^{3+} metal ions with high sensitivity.

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Structural Characterization and Biological Activity Study of Some Ligands and Their Vanadyl(IV) Complexes Based of Schiff Base

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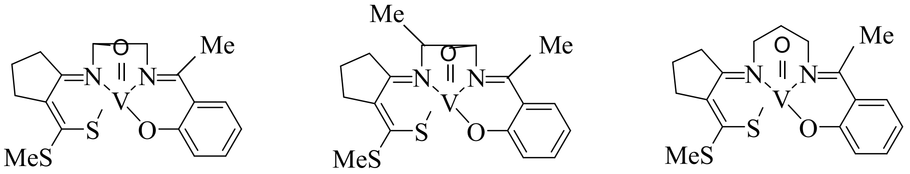
Keywords: Schiff base ligand, Oxovanadium complexes, Biological activity, Structural data.

With the increasing development of metallopharmaceuticals, numerous coordination compounds previously synthesized for purely laboratory purposes have become viable alternatives for therapeutic uses [1]. The ability of vanadium complexes to exhibit various oxidation states (III-V) and form stable complexes with biological properties makes them attractive in biology and medicine [2]. Three unsymmetrical Schiff bases derived from 2-hydroxy acetophenon were synthesized reacted with vanadium oxide acetylacetonate salt producing the corresponding complexes. The Schiff base oxidovanadium (IV) complexes were characterized physically as well as by using spectral characterization techniques including IR and UV–Vis spectroscopy, Mass spectrometry, powder XRD, EDX and elemental analysis. 1:1 metal:ligand stoichiometry has been proposed for $VO^{(IV)}$ complexes according to elemental analysis, energy dispersive X-ray analysis and Mass spectrometry. According to the spectrum data, the ligands behave as dibasic tetradentate chelating agent with NNOS donor atoms sequence toward central metal ion. All compounds have shown antibacterial activities against Staphylococcus aureus and Escherichia Coli, but the oxidovanadium (IV) complexes showed better activities as compared to the free ligand Schiff base.



Scheme1: Structure of oxidovanadium(IV) complexes.

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Synthesis of SBA-Pr-Is-MN-Py chemosensor for the detection of Hg^{2+} ions

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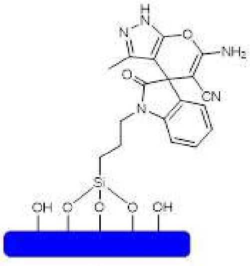
Keywords: SBA-15, Fluorescence spectroscopy, Hg^{2+}, Modification, Chemosensor

SBA-15 was chosen as an ideal scaffold for modification. This structure has outstanding features such as high porosity and large surface area, which has little absorption in the UV-Vis region. It can be easily modified with new organic chemical groups to produce new supports, which serve as chemosensor or absorbent of heavy metals. With the rapid growth of industry, heavy metal pollution, especially Hg^{2+} has become a serious threat to the environment. Current methods for detecting of these ions are usually expensive and complicated. Therefore, it is necessary to develop the sensitive and economic methods for the detection of Hg^{2+} ion. In this regard, the fluorescence sensors with high selectivity attracted the attention of researchers [1-3]. In this research, the surface of SBA-15 is modified with organic groups to produced SBA-Pr-Is-MN-Py, which acts as fluorescence chemosensor of Hg^{2+} ion (**Scheme 1**).



1
SBA-Pr-Is-MN-Py

Scheme 1: The structure of SBA-Pr-Is-MN-Py.

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Synthesis of SBA-Pr-Is-MN-EAOAc for the detection of Cu^{2+} ions

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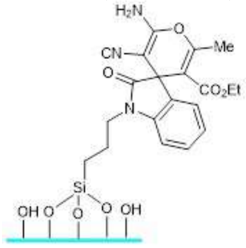
Keywords: SBA-15, Fluorescence, Cu^{2+}, Modification, Chemosensor

In 1998, Stuckey *et al*. succeeded in synthesizing SBA-15 with a regular structure and superior properties including non-toxicity, biocompatibility, and thermal stability. The modification of the porous structure of silica for the synthesis of organic-inorganic hybrid materials has been considered due to its unique properties such as increasing the adsorption capacity and selectivity in chemosensors. Also, SBA-15 is a suitable choice as an efficient nanostructure in the synthesis of modern fluorescence sensors due to its superior properties such as low cost, and surface reactivity. Cu^{2+} is know as an essential element for the human body, but its excessive consumption can be harmful. Therefore, the development of fluorescence chemosensor based on organic-inorganic hybrids for the detection of Cu^{2+} in the environment and the body is very important due to its simplicity and accuracy [1-3]. In this research, the surface of SBA-15 is modified with organic groups to produced SBA-Pr-Is-EAOAc, which acts as fluorescence chemosensor of Cu^{2+} ion (**Scheme 1**).



SBA-Pr-Is-MN-EAOAc

Scheme 1: The structure of SBA-Pr-Is-MN-EAOAc

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Investigation of catalytic activity of magnetic carbon quantum dots in 5-hydroxymethylfurfural production

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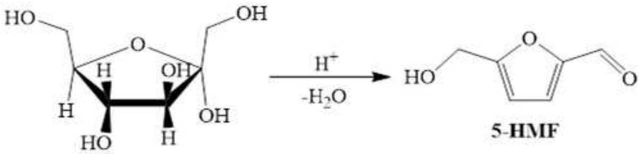
Keywords: CQDs, Catalyst, Magnetic nanocomposite, 5-hydroxymethylfurfural

As a novel carbon allotrope, carbon quantum dots (CQDs) have been investigated in various fields, including photocatalysis, bioimaging, optoelectronics, energy and photovoltaic devices, biosensing, and drug delivery owing to their unique optical and electronic properties [1,2]. In this study, a novel and heterogeneous CQD (carbon quantum dot) containing phosphorous acid functional groups was synthesized using citric acid, ethane-1,2-diamine, paraformaldehyde and phosphorous acid during two steps of reactions. Then, Fe_3O_4@CQDs-$N(CH_2PO_3H_2)_2$ nanocomposite was prepared and characterized by different techniques such as FESEM, EDS, VSM and TGA. Finally, the activity of Fe_3O_4@CQDs-$N(CH_2PO_3H_2)_2$ catalyst was investigated in the preparation of 5-HMF from fructose dehydration (Scheme1) in DMSO solvent [3]. With the purpose of finding the most appropriate conditions to achieve the highest yield of 5-HMF, several parameters such as time and the temperature of the reaction, the solvent type and the amount of catalyst were optimized.



Scheme1: Production of 5-HMF via fructose.

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Oxidation of dibenzothiophene using keggin-type Polyoxometalates as a model of desulfurization using hydrogen peroxide

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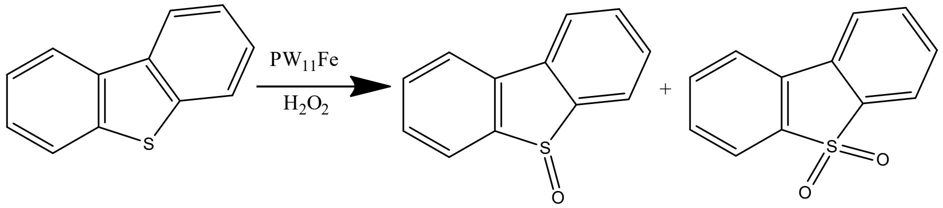
Keywords: Polyoxometalates, DBT, Green Chemistry

The tetrabutylammonium (TBA) salt of a Keggin-type polyoxometalate (POM), with the chemical formula $(TBA)_4[PW_{11}FeO_{39}].3H_2O$ was evaluated as a catalyst in the oxidation with hydrogen peroxide of dibenzothiophene (DBT), in acetonitrile with hydrogen peroxide at 60°C temperature [1]. Dibenzothiophene was oxidized to the corresponding sulfones with high conversion and selectivity. The stability and reusability of the catalyst were very high. The main factors affecting the desulfurization including temperature, catalyst/DBT molar ratio and H_2O_2/DBT molar ratio were investigated in detail [2]. The reaction rate increased with reaction temperature, Time, molar ratio catalyst and the molar ratio of H_2O_2. In this condition: DBT/ H_2O_2 /Catalyst Respectively 1/2/0.1 for 4h in 60 ˚C, we have oxidative removal of (DBT) 99.9 mol % [3].



Scheme 1: Desulfurization oxidation DBT using H_2O_2 and in presence $PW_{11}Fe$

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Ruthenium (0) nanoparticles supported nanostructured titanium dioxide as an active catalyst in hydrogen generation

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Keywords: Ru^0 nanoparticles, Titanium dioxide, Dehydrogenation, Dimethylamine borane

In this study, a nanostructured titanium dioxide substrate with high surface area was used to stabilize metal nanoparticles. Ru^0/TiO_2 nanoparticles were prepared by in situ reduction of Ru^{3+} ions adsorbed on titania nanopowder, and these nanoparticles were used as a catalyst for hydrogen production from ammonia borane (AB). Ruthenium is one of the early tested catalysts for this reaction and stands out for its high activity in catalytic H_2 generation from AB. AB is one of the high-hydrogen compounds which turns out to be a promising candidate for solid hydrogen storage. Ru^0/TiO_2 nanoparticles were prepared in two steps: first Ru^{3+} ions were impregnated from the aqueous solution on titania nanopowder, and then reduced by an aqueous solution of sodium borohydride. The prepared Ru^0/TiO_2 NPs were dried, bottled under inert N_2 gas atmosphere, and used for characterization by XRD (X-ray powder diffraction), TEM (transmission electron microscopy), ICP-OES (inductively coupled plasma optical emission spectroscopy) and XPS (X-ray photoelectron spectroscopy). The performance of the prepared catalysts in hydrogen release reactions and their recovery ability were examined.

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Photocatalytic Activity for Methylene Blue Degradation and Modeling by an Artificial Neural Network (ANN)

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Keywords: ANN, LSPR, Magnetic properties Nanocomposite, Photocatalyst

Finding new ways to remove contaminants is critical mission for scientists. In this research, Fe_3O_4/TiO_2/Ag magnetic nanocomposite synthesized for investigation of degradation of methylene blue (MB). Fe_3O_4 magnetic nanoparticles was first synthesized with simple co-precipitation method. Then the magnetic nanocomposite structure of Fe_3O_4/TiO_2 by hydrothermal method was shaped. After that, to improve the ability of the nanocomposite to reduction of MB, Ag nanoparticles was doped on the surface of the Fe_3O_4/TiO_2. In fact, in this structure, we used local surface plasmon resonance (LSPR) future of Ag and photocatalyst property of TiO_2 to modify the ability of MB reduction [1]. The results show that the nanocomposite formed successfully in desired structure and morphology. Catalytic measurements on the samples show an excellent efficiency for the MB degradation. After the reduction of MB, one can use a magnet bar to separate the catalyst from solution easily. Artificial neural network (ANN) models can eliminate the huge part of experimental investigations in various filed of science and technology [2]. After gathering some information about the methyl blue degradation, the ANN modeling was carried out to calculate the optimum values of initial variables to achieve the maximum removal efficiency. In this project, we used an initial ion concentration, the amount of nanocomposite that were used in photocatalyst activity and removal time as initial variables, finally the removal efficiency of pollution (MB) was considered as the output. In this project, we used a genetic algorithm (GA) to trained models and predation

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Synthesis and characterization of Ni (II) complex as an effective catalyst for aldehyde to amide conversion

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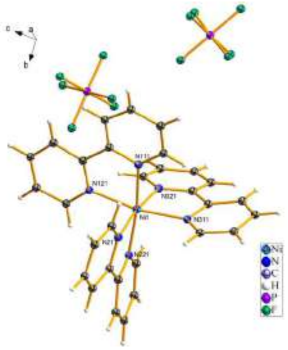
Keywords: Ni(II) complex, Catalyst, Aldehyde, Amid

Chemical synthesis plays a crucial role in advancing numerous scientific fields, ranging from material science to pharmaceuticals[1]. Transition-metal-catalyzed reactions offer widely applicable techniques for creating and developing new molecules that are useful across various applications [2]. Despite their utility, these modern methods often rely on pre-functionalized starting materials to achieve control over chemo- and regio-selectivity.

A Ni(II) complex, $[Ni(bpy)_3]PF_6$, (**Scheme1**) was prepared by reacting bpy with $Ni(NO_3)_2.6H_2O$ in a methanol solution [3]. Additionally, the catalytic effect of this complex was screened for the conversion of aldehydes to primary amides. Various factors, including reaction time, solvent, base, and catalyst loading, were investigated.



Scheme1: Crystal structure of $[Ni(bpy)_3](PF_6)_2$.

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NiFe Oxide-Based Electrodes Loaded on Indium Tin Oxide as Effective Electrocatalysts for Oxygen-Evolution Reaction

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Keywords: Indium tin oxide, Electrocatalyst, Energy storage, Tafel plot

The oxygen-evolution reaction (OER) is a vital process in energy storage applications such as metal-air batteries and water splitting [1,2]. NiFe oxide-based electrodes have gained significant attention for OER due to their promising features [3]. In this study, we investigated the effectiveness of NiFe oxide loaded on indium tin oxide as an electrocatalyst for OER in the presence of $NaHCO_3$.

The electrocatalyst was characterized using various techniques, including Raman spectroscopy, diffuse reflectance spectroscopy (DRS), X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectrometry (EDX). Our findings revealed that NiFe oxide loaded on indium tin oxide serves as an effective and durable electrocatalyst for OER in the presence of $NaHCO_3$.

Furthermore, our results suggest that the electrolysis of $NaHCO_3$ solution offers a highly promising alternative for producing oxygen and hydrogen compared to corrosive acidic or alkaline solutions. These findings demonstrate the potential of NiFe oxide-based electrodes for OER and offer insights into developing sustainable and efficient energy storage systems.

The Tafel plot reveals a linear correlation between the logarithm of current density (log(j)) and overpotential, with a Tafel slope of 59.2 mV/decade. Notably, the onset of WOR, depicted in the Tafel plot, occurs at 1.60 V (overpotential: 370 mV).

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Co(II) “end-off” homo-dinuclear complex as a functional mimic of phenoxazinone synthase enzyme

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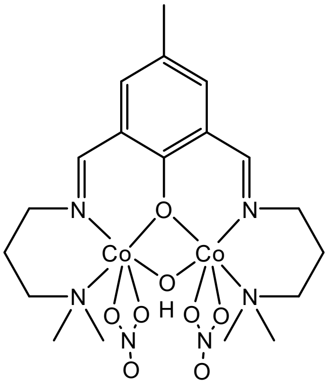
Keywords: Cobalt(II) Schiff base complex, Homo-dinuclear complex, Phenoxazinone synthase

In this research, a dinuclear complex of Co(II) was synthesized and characterized by FT-IR, UV-Vis spectroscopy, elemental analyses and single crystal X-ray crystallography techniques. As shown in the **Scheme 1**, an “end-off” Schiff base ligand 2,6-bis{3-(dimethylamino)-propyliminomethyl}-4-methylphenol with $(NN)_2O$ coordination site coordinated to Co(II) metal centers and an internal phenoxo bridge and an external hydroxo bridge are placed between the two metal centers [1]. The enzymatic activity of this complex as a model of phenoxazinone synthase was investigated by UV-Vis spectroscopy. The catalytic constant ($k_{cat} = 0.66$ min^{-1}) showed the proper efficiency of this complex as a phenoxazinone synthase model.



Scheme1: Co(II) complex structure.

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Immobilized Cu(II) Schiff base complex on MGO, a green approach for olefin oxidation

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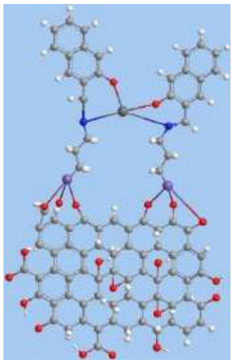
Keywords: Magnetic Graphene Oxide (MGO), Schiff base, Oxidation, Olefin, Catalyst

Magnetic Graphene Oxide (MGO) has been attracting much interest as a heterogeneous catalyst upon grafting with the Schiff base complex. Magnetic properties of MGO can enable easy recovery of the catalyst and hence promise in catalytic applications.[1,2] MGO surface modification by organosilane groups is allowed to graft Schiff base complex.[3] The ligand was synthesized through the nucleophilic attack between (3-Aminopropyl)trimethoxysilane and 2-hydroxynaphthalin-1-carbaldehyde followed by complexation with Copper(II) acetate. Characterization was done using FTIR, XRD, EDS, and SEM. The Schiff base complex grafted on MGO exhibited 95% conversion of the oxidation of styrene into benzaldehyde, benzofuran and other byproducts by using H_2O_2 as a green oxidant.



Scheme 1: Overall view of Schiff base complex grafted on MGO.

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Copper(II) complex with compartmental ligand: Synthesis, characterization and DNA binding

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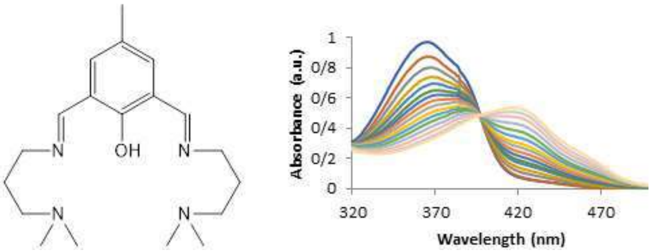
Keywords: Schiff base complex, Cu(II) complex, DNA binding, Compartmental ligand

In this study, homo-dinuclear Copper(II) complex with an “end-off” compartmental Schiff base ligand 2,6-bis{3-(dimethylamino)-propyliminomethyl}-4-methylphenol (**Scheme 1, left**) was synthesized and characterized. This dinuclear complex has an external hydroxo bridge and an internal phenoxo bridge. DNA is the main target in cancer treatment. Examining the drug interaction with DNA is important in this sense. So far, the interaction of many complexes with DNA has been studied [1, 2]. The binding of the complex with FS-DNA was investigated using circular dichroism, UV–Vis spectroscopy and molecular docking and deduced that “intercalation” is the main mode of interaction with FS-DNA (**Scheme 1, right**).



Scheme 1: Structure of the ligand (left). Absorption spectra of Cu(II) complex with different concentrations of FS-DNA (right).

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Synthesis, characterization and DNA interaction of homo-dinuclear Schiff base cobalt(II) complex

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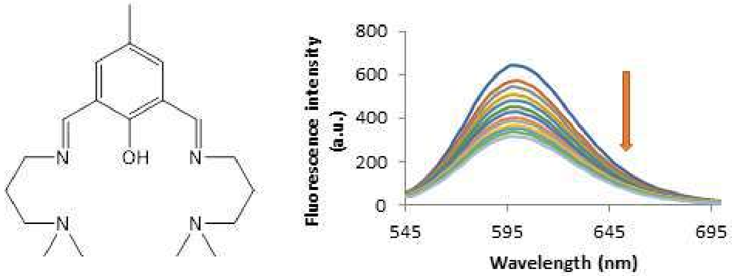
Keywords: Cobalt(II) complex, DNA binding, Schiff base complex, Dinuclear complex

The study involved the synthesis and characterization of a homo-dinuclear Cobalt(II) complex with a multidentate Schiff base ligand (2,6-bis{3-(dimethylamino)-propyliminomethyl}-4-methylphenol) (**Scheme 1, left**). This complex exhibit propensity to interact with DNA, which is significant in cancer treatment research. The interaction of various complexes with DNA has been studied extensively [1,2]. In this study, the binding of the complex with FS-DNA was investigated using various techniques (**Scheme 1, right**), and it was found that the main mode of interaction was "intercalation".



Scheme 2: Structure of the ligand (left). Fluorescence spectra of FS-DNA/EtBr with different concentrations of Co(II) complex (right).

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Ag/Fe_3O_4/SiO_2@MWCNTs: As an Efficient Reusable Magnetic Nano-catalyst for the Green Synthesis of New Imidazopyrimidine Derivatives via One-Pot Multicomponent Reactions

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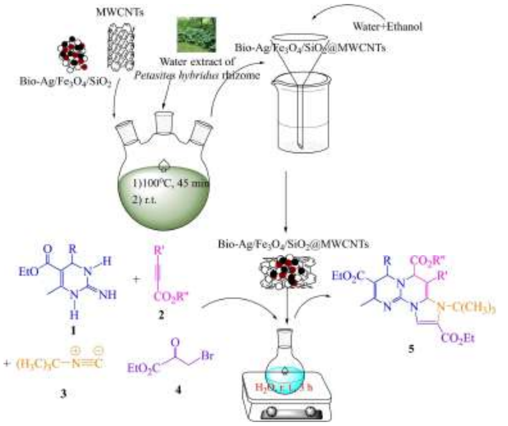
Keywords: Activated acetylenic compounds, Imidazopyrimidines, Multicomponent reaction

Heterocyclic compounds with spiro moiety are significant because of their inflexibility and important biological properties. The heterocyclic compounds among organic compounds are well-known for showing many biological properties. One strategy for the creation of heterocyclic compounds is a multicomponent reaction (MCRs), which could produce these compounds with significant biological activity in one pot and high yields compared with reactions with more stages. MCRs relative to multi-step reactions have some advantages such as good efficiency of the product, simple deletion of them, and having atom economic and low reaction time. Ag/Fe3O_4/SiO_2@MWCNTs MNCs magnetic nanocomposites as an effective catalyst were employed for generating imidazopyrimidine derivatives in high yields. The structure of the synthesized nanocatalyst was confirmed by SEM, XRD, TEM, VSM, EDX, and XPS analysis. These new compounds were synthesized by using the multicomponent reaction of cyclic guanidine derivatives, electron-deficient acetylenic compounds, tert-butyl isocyanide, ethyl bromopyruvate, and synthesized nanocatalyst in aqueous media at room temperature. It should be mentioned that the high performance of the nanocatalyst was synthesized by using water extract of *Petasits hybridus* leaves, which was utilized in these reactions for many times to confirm the reusability of the nanocatalyst (**Scheme1**).



Scheme1: Synthesis of new derivatives of imidazopyrimidine.

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Structural and computational studies on coordinated tetrafluoroborate complexes of rhenium tricarbonyl bearing two bidentate nitrogen donor ligands

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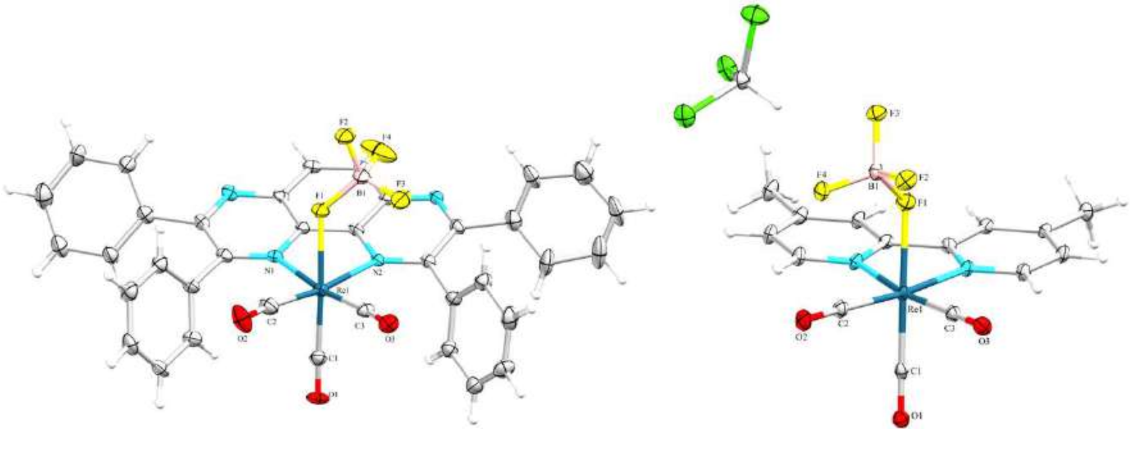
Keywords: Weakly coordinated anion, X-ray diffraction, n → π* interaction, Molecular interactions, Halogen bonding

The complexes *fac*-[$Re(CO)_3(NN)(FBF_3)$] {*NN* = 4,4'-dimethyl-bipyridine (4,4'-Me_2bpy) (**1**) & 2,3,6,7-tetraphenyl-1,4,5,8-tetraazaphenanthrene (Ph_4TAP) (**2**)} are formed by abstraction reaction of the respective chloro-complexes with $AgBF_4$ in dry dichloromethane [1]. The tetrafluoroborate complexes were characterized and their solid-state structures were determined by single-crystal X-ray diffraction. The intra- and intermolecular interactions were theoretically studied by QTAIM, non-covalent interaction index-independent gradient model (NCI-IGM), and natural bond orbital (NBO) approaches. The interaction energy of the coordinated tetrafluoroborate anion fragment with [$Re(CO)_3$(4,4'-Me_2bpy)] and [$Re(CO)_3$(Ph_4TAP)] complex cation fragments were done by energy decomposition analysis with the combination of the natural orbital for chemical valence (EDA–NOCV) analysis scheme. The complexes showed interesting intramolecular n (F_{BF4}) → π* (C≡O) interactions between the coordinated BF_4^- and equatorial carbonyl ligands. The crystal packing also showed intermolecular n → π*, C−H···O, C−H···F, F···F interactions and O···Cl halogen bonding [2] **(Scheme1)**.



Scheme1: ORTEPs of complex1 (right) and complex2 (left).

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High Capacity Arsenate Removal Using Dihydrotetrazine Decorated Zirconium-Based Metal-Organic Frameworks

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Keywords: zirconium metal-organic frameworks (Zr-MOFs), dihydrotetrazine, arsenate (AsO43-), hydrogen bonding

Zirconium metal-organic frameworks (Zr-MOFs) are potential candidates for decontamination of water resources from harmful pollutants due to their modulable porosity and chemical stability in aqueous solutions. Linker functionalization is an approach for tuning the host-guest-chemistry of Zr-MOFs and extend their applications in environmental monitoring. In this work, the structure of UiO-66(Zr) (formulated Zr6(OH)4O4(BDC)6, BDC2- = benzene-1,4-dicarboxylate) was functionalized with dihydrotetrazine group via post-synthesis linker exchange (PSLE) method. The functionalized framework, UiO-66(Zr)-DHTZ, was applied for the removal of arsenate ions from aqueous solutions. The results show that UiO-66(Zr)-DHTZ can adsorb 583 mg.g-1 of As(V) at pH = 7 after 2 hours which is significantly higher that the UiO-66(Zr). According to X-ray photoelectron spectroscopy (XPS) and Fourier-transform infrared (FTIR), the removal mechanisms is based on possible hydrogen bindings between free –C–NH and –C=N sites of dihydrotetrazine function with –OH and –O- sites of As(V) species. Removal tests in real-samples show that UiO-66(Zr)-DHTZ still has high capacity (220 mg.g-1) to As(V) ions in complex matrixes and also can decrease the concentration of As(V) below detection limit (0.05 ppm) of inductively coupled plasma optical emission spectroscopy (ICP-OES) method. This work is indicative of the fact that rationally functionalized Zr-MOFs can be considered as potential candidates for water treatment in real-life applications.

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The n → π* Interactions in Metal-Carbonyl Complexes: A Case Study on $Re(CO)_3$ Core Complexes

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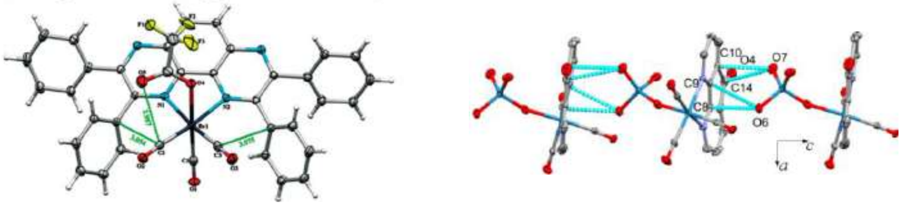
Keywords**:** Non-covalent Interactions, Bürgi-Dunitz Trajectory, Intramolecular Interactions

Noncovalent interactions are of key importance in numerous chemical and biological processes and in materials science. Among the noncovalent interactions which are the basis of supramolecular chemistry, those involving lone pair···π-systems (lp···π) are of great importance in both chemistry and biology. The occurrence of such an interaction was reported first by Bürgi *et al*. in the structural study of (*S*)-methadone in which the nucleophilic dimethylamine segment moves close to the carbonyl group. Following the observation of this significant structural feature, they proposed a geometrical reaction pathway for compounds containing nucleophilic and electrophilic centres in which the reaction coordinates could be mapped along a minimum energy pathway, the so-called Bürgi-Dunitz trajectory [1].

Allen, Raithby and co-workers in 1998 and 2006, respectively, reported the first systematic CSD and computational studies of carbonyl···carbonyl interactions in organic compounds and first-row transition metal complexes. In 2011 and 2012, Zukerman-Schpector *et al*., highlighted the importance of the intermolecular metal-carbonyl···π(aryl) interactions as a supramolecular synthon for the stabilisation of transition metal carbonyl crystal structures [2]. In 2018, Echeverria noticed the importance of n → π* in metal carbonyl complexes and studied them by computational approaches [3] (**Scheme1**).



Scheme1: The ORTEP of two $Re(CO)_3$ complexes bearing NN-donor ligands.

In this presentation, the noncovalent interactions in a series of metal carbonyls complexes with focus on the participation of n → π* in their molecular structure and crystal packing will be discussed.

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Drug Delivery Using Hydrophilic MOFs: Effect of MOFs Structure Properties on Biological Behavior of Carriers

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Keywords: Metal-organic frameworks, Drug Delivery, Nimesulide, Cancer

To investigate how the pore structure of metal–organic frameworks (MOFs) affects drug adsorption and delivery, we created two MOFs, TMU-6(RL1) and TMU-21(RL2), featuring amine-based N-donor pillars with phenyl or naphthyl cores and varying hydrophilic characteristics. We characterized these MOFs using TG, IR, XPS, and PXRD techniques, revealing their high adsorption efficiency, stability, and controlled release. Nimesulide (Nim), an anticancer drug, was adsorbed through multiple mechanisms, including Hostπ–πGuest interactions and hydrogen bonds. Hirshfeld surface analysis indicated that switching from a benzene to a naphthalene core reduced $\pi\cdots\pi$ and N···H interactions in TMU-21(RL2) but increased interactions with guest molecules. These findings suggest that altering MOF hydrophobicity/hydrophilicity influences Nim adsorption capabilities. In vitro studies demonstrated that Nim in MOFs@Nim composites exhibited significantly greater cytotoxicity against HeLa and HT-29 cancer cells compared to free Nim. Overall, the biological behavior of the carriers can be fine-tuned by modifying the structural properties of MOFs. (**Scheme1**).

Scheme1: Preparation of MOFs and drug loading process

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Chitosan coated magnetic nanoparticles in adsorption of Cd(II) micropollutant

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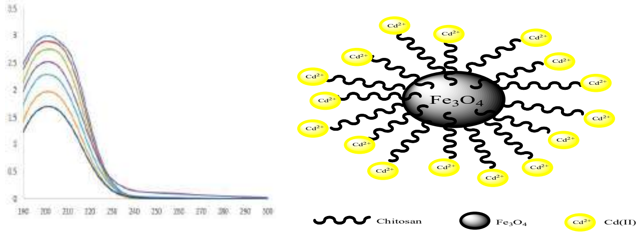
Keywords: Chitosan, Iron oxide nanoparticles, Cd(II), Adsorption capacity

The current work reports synthesise and characterization of chitosan coated iron oxide nanoparticles (CS-Fe_3O_4) and investigation in its capacity for removing cadmium ions micropollutant from wastewater. We synthesized the CS-Fe_3O_4 by coating chitosan onto the surface of iron oxide nanoparticles using the in situ coating method [1]. The influencing parameters including initial concentration and contact time were evaluated and optimized. The electrostatic attraction may form between the negatively charged functional groups such as -COO- and -O- on the surface of CS-Fe_3O_4 and Cd(II) ion [2]. Therefore, the adsorbents exhibited a high adsorption capacity for Cd(II) ion under the action of both coordination bonds with the oxygen atom in Fe_3O_4 and electrostatic attraction [3] (**Scheme1**). Effects of initial Cd(II) concentration (30, 60, 90, 100, 120 and 140 mg/L) on the adsorption of Cd(II) onto CS-Fe_3O_4 nanoparticles were investigated at room temperature. The adsorption of Cd(II) ions by CS-Fe_3O_4 nanoparticles increased with the increasing the initial concentrations of ions. The highest absorption capacity of 130.6 mg/g was obtained at initial concentration of 140 mg/L. The effect of contact time on the adsorption of Cd(II) by CS-Fe_3O_4 shows that the removal efficiency increases with increasing time. The Cd(II) removal efficiency received to 88.33% over a period of 120 min.



Scheme1: The schematic illustration of the related adsorption mechanisms of CS-Fe_3O_4 toward Cd(II).

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Application of a dehydrogenated ferrocene-based azine in designing multichannel sensors for detecting some metal ions

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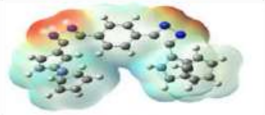
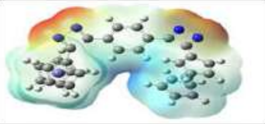
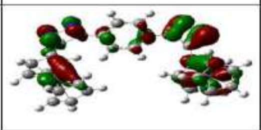
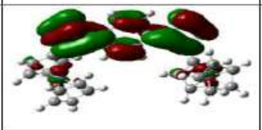
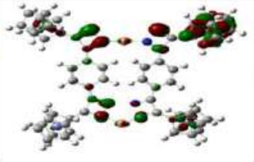
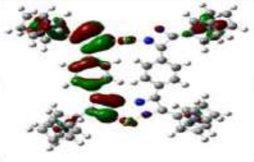
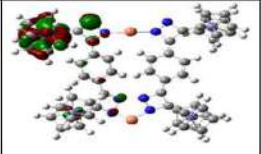
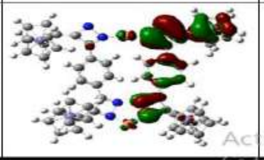
Keywords: Azine, Ferrocene-based azines, Multichannel sensors, Metal ion detection, DFT

Ferrocene-based azines have emerged as significant compounds in chemical sensors for metal ion detection, displaying unique properties ideal for designing multichannel sensors with high sensitivity and selectivity.[1] Since these compounds would be suitable sensors for the detection of heavy metal ions in the environment, a computational study was carried out using a DFT approach to investigate the activity of an "unsymmetrical ferrocene-based double azine"[2] after its dehydrogenation and the interaction with various metal cations in both gas and solvent phases. Optimized geometries and corresponding molecule orbitals (MOs) energies for Cu(II), Zn(II), and Co(II) complexes were helped by the Gauss View 6.0 visualization software at the B3LYP level, and 6–311++ G(d,p) basis set for non-metal elements (C, H, N, O) and LANL2DZ basis set for metal ions were treated. Some results are listed in Scheme 1.

Scheme 1: presents some optimized studied structures and E_{homo} & E_{lumo} in gas and solvent phases

Structure	ESP	HOMO	E_{HOMO} (eV)	LUMO	E_{LUMO} (eV)	E_{gap} (eV)
Ligand (gas)			-6.04		-3.39	2.65
Ligand (solvent)			-6.01		-3.53	2.48
L-Cu (gas)			-13.14		-12.88	0.26
L-Cu (solvent)			-6.39		-5.31	1.07

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Synthesis of a new nanomagnetic hybrid of MOF-COF and its application in alcohols oxidation

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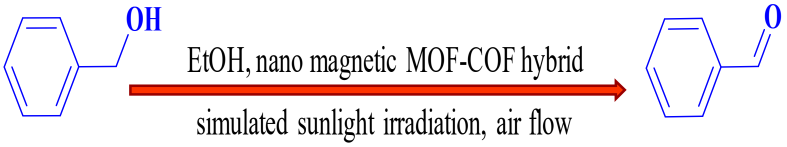
Keywords: Metal-organic framework, Covalent-organic framework, Hybrid, Nano magnetic

A novel nanomagnetic hybrid of MOF and triazine based COF was synthesized by the hydrothermal method*(1)* and characterized by FT-IR, XRD, DRS, FE-SEM, EDX-maping, XPS and TGA. This catalyst was used as a new heterogeneous photocatalyst for air the oxidation process of alcohols to aldehyde derivatives under simulated sunlight radiation*(2)*. The hybrid photocatalyst has a lower band gap and enhanced catalytic activity compared to each of the individual components, indicating the synergistic effect of the MOF and COF*(3)*. The good reusability, high efficiency without any additives, make this method as an environmentally friendly process for the preparation of these important scaffolds. (**Scheme 1**).



Scheme 1: Photocatalytic air oxidation of benzyl alcohols to aldehydes catalyzed by a new MOF-COF hybrid

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Photoinduction effect in photocatalytic degradation of phenol under visible light

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Keywords: Phenol solution, photocatalytic degradation, ZnO

ZnO nanoparticles were impregnated with merbromin dye and used as visible light active photocatalysts for degradation of phenol. UV–Vis spectral changes of phenol solution over time during photocatalytic degradation using the merbromin -ZnO (M-ZnO) under optimal conditions (**Figure 1**) reveals the percentage of phenol degradation reached 100% with M-ZnO during a 240-minute study. However, this modified photocatalyst material exhibited the well-known photoinduction effect which refers to an increase in absorbance intensity of pollutant during a certain period of initiation of photocatalytic reaction instead of decrease. As can be seen in Figure 1a, during the photocatalytic degradation of phenol on the surface of M- ZnO, an increase in absorbance intensity is observed after dark stirring stage, while phenol solution is concomitantly exposured to visible light and photocatalyst. This trend persists for a certain duration during the photodegradation process. This behavior, in which the concentration of the pollutant rises relative to that observed at previous sampling times, is referred to as the photoinduction period. This effect has been frequently reported in the photodegradation of phenolic compounds, particularly during the hydroxylation stage, where the involvement of free radicals has been noted. The phenomenon of the photoinduction period contributes to a slower reaction rate [1].

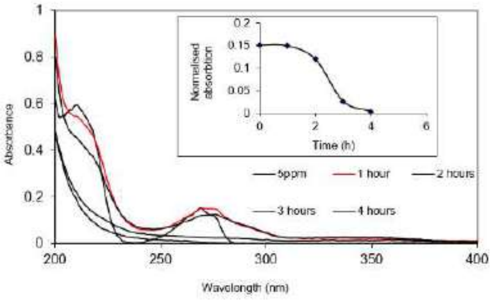

Figure 1: UV–Vis spectra of phenol solution during photocatalytic degradation on M-ZnO.

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Design and DFT study of new nano buds from the combination of C60 fullerene and nanobowl.

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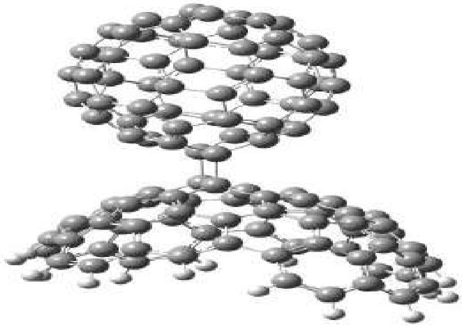
Keywords: Molecular design, DFT, NLO

In this research, new Nano buds are designed from the combination of fullerene C60 and Nano bowls. all calculations were perform using the Gaussian 09W package.The structure, electrical properties and optical properties of the designed nanostructures were calculated. It was shown that all structures do not have imaginary frequency and may have stable structures. The cohesive energies of the designed Nano buds were calculated, which high cohesive energies may be another evidence of their stability. Population analysis was performed to estimate the relative population of Nano buds and it was shown that configuration E is the dominant population. The nonlinear optical properties of the designed molecules were calculated and compared with the parent molecules, and a high improvement in NLO properties was observed in all Nano bud configurations [1-3].



Scheme1: The optimal structure of primary nanostructures and nanobuds.

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Adsorption of Deep Eutectic Solvents on Pristine and Mono-*Vacancy Defected* Boron-Nitride Nanotubes: A DFT Study

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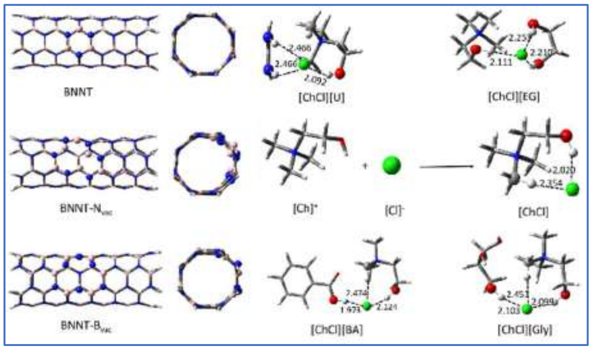
Keywords: Boron nitride nanotube, Deep eutectic solvent, Noncovalent interaction, DFT

The physical properties of Boron nitride nanotubes (BNNTs), consisting of interlocking six-membered B_3N_3 rings in the ideal, can change through solvent-surface interactions [1]. The absorbed solvent molecules, making up a significant amount of the material's mass, act as an extension of nanomaterials and effectively tune the nanomaterials' properties adjusting their functionality for various applications. Recently, deep eutectic solvents (DESs) have received much attention for their ability to exfoliate nanomaterials. In this study, Density functional theory (DFT) calculations are performed using Gaussian 09 D.01[2] suite of programs at the M06-2X/cc-pVDZ level of theory to evaluate the intermolecular interactions between four common choline chloride ([ChCl])-derived DESs and pristine and defective BNNTs. [ChCl] is the hydrogen bond acceptor (HBA) and is paired, in turn, with four hydrogen bond donors (HBDs): urea ([U]), ethylene glycol ([EG]), glycerol ([Gly]), or benzoic acid ([BA]) (**Scheme 1**). Our calculations revealed that the DESs spontaneously adsorb onto the nanotubes through van der Waals (vdW) interactions and charge transfer occurs from the DESs to the nanotubes; affinity is far higher for nanotubes with a boron vacancy. Adsorption of DESs onto BN is stronger than onto carbon nanotubes. DESs incorporating benzoic acid show far stronger interactions with the surfaces due to possible π-π interactions, unavailable to the other DESs.



Scheme 1: The M06-2X/cc-pVDZ optimized geometries of nanotubes and the most stable geometry of DESs.

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Investigating the Adsorption Mechanism of Known Deep Eutectic Solvents on Carbon Nanotubes: A DFT Study

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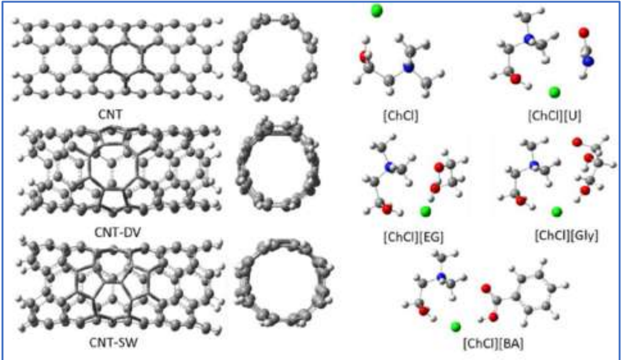
Keywords: Carbon nanotube, Stone-Wales defects, Double-vacancy defects, Deep eutectic solvents

In recent decades, deep eutectic solvents (DESs) have gained recognition as a practical substitute for conventional volatile solvents, attributed to their overall cost efficiency [1]. DESs play a significant role in the exfoliation of carbon nanotubes (CNTs) due to their unique properties. They can achieve superior dispersion of CNTs by overcoming strong π–π stacking interactions. Understanding the adsorption mechanism of DESs on the CNTs is fundamental to advancing the development of new materials and technologies in various fields, including electronics, energy storage, and catalysis. In this study, density functional theory (DFT) calculations were conducted using Gaussian 09 D.01 [2] suite of programs at the M06-2X/cc-pVDZ level of theory to explore the interactions between DESs and the surfaces of pristine carbon nanotubes (CNT), double vacancy CNT (CNT-DV), and single-walled CNT (CNT-SW). The DESs under investigation are composed of choline chloride ([ChCl]) serving as a hydrogen bond acceptor (HBA) and various hydrogen bond donors (HBDs) including urea ([U]), ethylene glycol ([EG]), glycerol ([Gly]), and benzoic acid ([BA]) (**Scheme 1**). Noncovalent interaction (NCI) plots indicate that the adsorption of these DESs onto the surfaces is primarily facilitated by van der Waals (vdW) forces. Energy decomposition analysis (EDA) shows that the contribution of dispersion interactions to the adsorption process is significantly higher than that of electrostatic and orbital interactions.



Scheme 1: The most stable geometries of the CNT, CNT-DV, CNT-SW, [ChCl], [ChCl][U], [ChCl][EG], [ChCl][Gly], and [ChCl][BA] as calculated using M06-2X/cc-pVDZ.

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DFT investigation of a Zn-doped carbon nanocone for the drug delivery of methylated aspirins

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Keywords: Nanocarbon, Complexation, Aspirin

The models of original aspirin (ASP) and eight methylated derivatives (A1-A8) were obtained from the ChemSpider structural bank [1]. The singular models were optimized to obtain the stabilized structures, which were confirmed by the evaluated real vibrational frequencies of infrared (IR) spectra. Next, each of the ASP and A1-A8 models were combined with the Zn-doped carbon nanocone (NANO) substance for examining the formations of ASP@NANO complexes (Fig. 1). As a consequence, nine models of bimolecular complexes were stabilized and their global minimizations were confirmed by the evaluated real vibrational frequencies of IR spectra. Subsequently, structural and electronic descriptors were evaluated for the optimized singular and bimolecular models to assess their physical and chemical features. By the important roles of frontier molecular orbitals for defining molecular electronic features, quantities of energy levels of the highest occupied and the lowest unoccupied molecular orbitals (HOMO and LUMO) were evaluated. Additionally, representations of electrostatic potential (ESP) surfaces and diagrams of density of states (DOS) were exhibited for the investigating models . Moreover, the values of quadrupole coupling constants (Cq) were calculated for the oxygen and zinc atoms to show chemical environments of the dominant interacting atoms of ASP and NANO models in the singular and bimolecular states. The current calculations were performed using the B3LYP exchange–correlation functional and the 6-31G* basis set as implemented in Gaussian program [2].

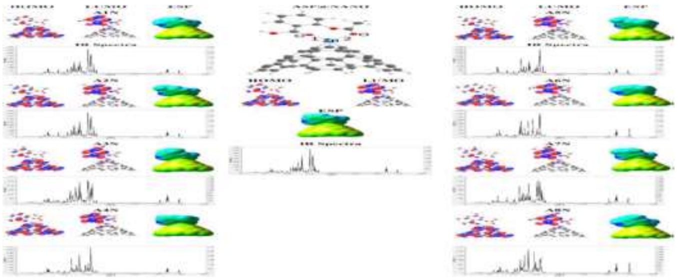

Fig. 1. Representations of bimolecular.

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Application of Metal Organic Framework as Sorbent to Extraction and Preconcentration of Pesticide

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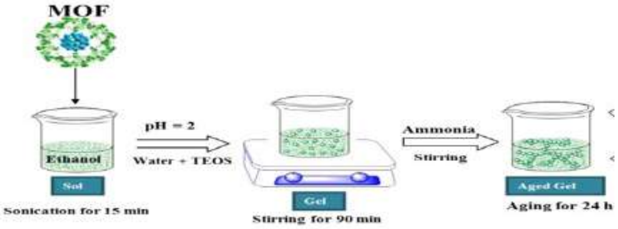
Keywords: Metal Organic Framework, Pesticide, silica aerogel, SPME

Silica aerogels (SAs) are light solids with high porosity, low density, low thermal conductivity, and high surface area. Because of their particular properties, SAs have found many applications in drug delivery, thermal insulators, sensors, and extraction methods. MOFs as crystalline materials have found increasing attention because of their individual properties [1]. The existence of a metal cluster and an organic compound as linker leads to porous with adjustable pore and high surface area structure. Thus, they are used in various applications such as gas separation and storage, catalysis, and sample preparation methods such as solid phase extraction and solid phase microextraction of different organic compounds. A new hybrid of silica aerogel with MIL-101(Fe) metal–organic framework was prepared and used as a highly porous fiber coating for headspace solid-phase microextraction of Pesticide. Applying a permanent magnetic field to the sorbent increased the extraction efficiency [2]. Optimization of the extraction parameters was carried out using a GC–MS instrument. The prepared fiber was stable in multiple injections with good relative standard deviations for 5 replicates. The proposed method was successfully applied to the extraction and identification of pesticide of some soil samples.



Scheme 1: Schematic of preparation of silica aerogel with MIL-101(Fe)

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Copper, Silver and Gold extraction from printed circuit boards (PCB) using electrochemical methods

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Keywords: Electronic waste, Metal extraction, Electrowinning

The global generation of electronic waste has surged dramatically over the past few decades, making it one of the fastest-growing categories of solid waste. Electronic waste, or e-waste, refers to electrical and electronic devices that have reached the end of their useful life [1,2]. The rising demand for advanced electronic devices contributes to the annual production of millions of tons of e-waste, which contains significant amounts of both basic and precious metals, including copper, gold, and silver.

Currently, the world produces between 40 and 50 million tons of electronic waste each year, with this figure increasing by approximately 5 million tons annually. Various methods exist for processing and recycling e-waste, such as disposal and incineration; however, these approaches often present significant economic and environmental drawbacks [3]. To achieve effective and sustainable recycling of e-waste, robust infrastructure and coordinated programs are essential. Reusing recycled materials can conserve energy and raw materials while significantly enhancing the circular economy in developing countries.

Today, numerous researchers are focused on extracting valuable elements from electronic waste and are proposing various innovative solutions [1-3]. Among these, chemical and electrochemical methods stand out as environmentally friendly alternatives. This research aims to explore the electrochemical deposition techniques for separating copper, gold, and silver from e-waste and to identify optimal conditions for these processes.

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Ligand Induced Intramolecular Cuprophilic and Argentophilic Interactions in Bimetallic Cu(I) and Ag(I) Phosphine Complexes and Assessment of their Anti-tyrosinase and Anti-bacterial Effects

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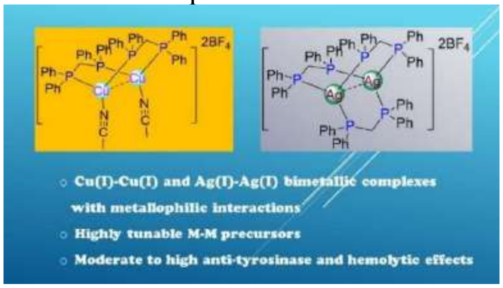
Keywords: Cuprophilic interactions, Metallophilic interactions, Phosphine Complexes

Binuclear silver(I) and copper(I) complexes, 1 and 5, with bridging diphenylphosphine ligands were prepared. In 1, the silver(I) center is located inside a trigonal plane composed of three phosphorus donors from three separate and bridging dppm ligands. The fourth coordination site is filled with neighboring silver(I) ions. The short Ag…Ag distance, as a result of small bite angles from bridging dppm ligands, was determined to be 2.9463(4) Å. In 5, the Cu…Cu distance is 2.915(6) Å, significantly shorter than that observed in comparable structures. Derivatization of 1 and 5 using selected sulfur donor dialkyldithiophosphates gave eight novel heteroleptic binuclear complexes. Single crystal X-ray diffraction studies of five of these complexes revealed interesting structural features including strong metallophilic interactions in 1 and 5 and multiple intramolecular and intermolecular hydrogen bonding interactions. The antibacterial activities of complexes were also screened against gram-positive (Staphylococcus aureus PTCC 1112) and gram-negative (Escherichia coli PTCC 1330) bacteria. Anti-tyrosinase and hemolytic effects of the selected compounds were also determined. Time-dependent density functional theory (TD-DFT), Interaction Region Indicator (IRI), and Fuzzy Atom Bond Order (FBO) analyses of the selected complexes provided insights into the electronic and structural characteristics of the metal complexes.



- Cu(I)-Cu(I) and Ag(I)-Ag(I) bimetallic complexes with metallophilic interactions
- Highly tunable M-M precursors
- Moderate to high anti-tyrosinase and hemolytic effects

Scheme 1: Synthesis of binuclear Cu(I) and Ag(I) complexes.

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Application of Metal Organic Framwork as Sorbent to Extraction and Preconcentration of Phenobarbital

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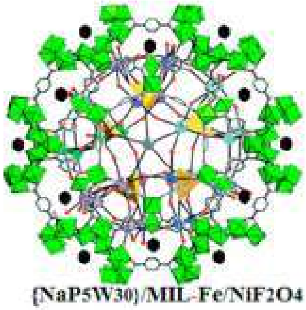
Keywords: Metal Organic Framwork, Phenobarbital, Extraction, magnetic solid-phase extraction

Polyoxometalates (POMs) are metal-oxygen macro anion cluster adsorbents known for rich structure, adjustable acidity, high thermal stability, and reversible redox properties. Therefore they can beused in different fields such as analytical chemistry, medicine, and homogeneous and heterogeneous catalysis [1]. MOFs, as a type of crystalline nanomaterial, can be produced through the self-assembly process of clusters/metal ions and organic linkers. As a result of their specific characteristics like vast surface area high porosity, tunable pore size, simple preparation process, high stability, tailored chemical functionalities, flexibility, and diverse topology, MOFs have gained much attention recently. In this work, {NaP5W30}/MIL101-Fe/NFO) was used as sorbent for magnetic solid-phase extraction method based on agarose coated magnetic nanoparticles coupled to a magnetic field agitation used for the preconcentration of Phenobarbital [2] (**Scheme1**).



Scheme1: Structure of NaP5W 30}/MIL101- Fe/NFO nanocomposite.

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Modified lignin-supported copper complex: A magnetically separable and reusable catalyst for the synthesis of *N*-sulfonyl-*N*-aryl tetrazoles

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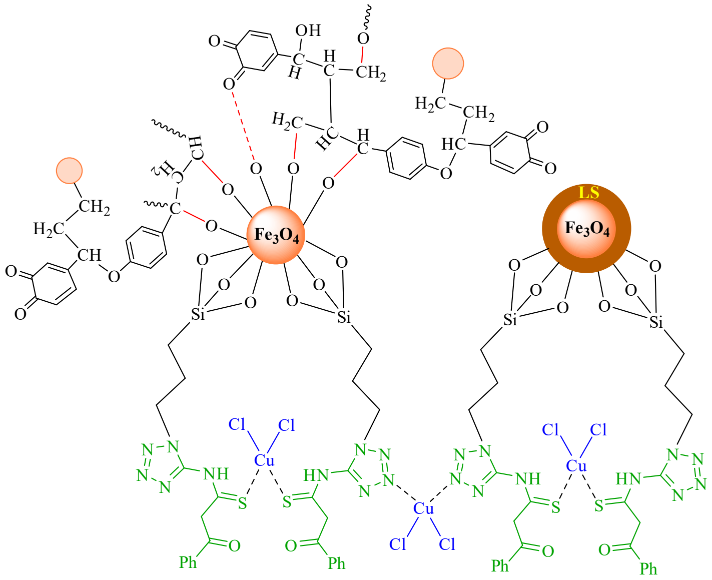
Keywords: Lignin, copper complex, tetrazole, *N*-((1*H*-tetrazol-5-yl)carbamothioyl)benzamide

Tetrazoles are an important class of synthetic organic *N*-heterocyclic molecules with an extensive range of applications, especially in catalysis [1]. Among the available supports, biopolymers such as lignin are used to immobilize metal nanoparticles (NPs) or complexes due to their excellent stability, low cost, and high surface area [2]. In this study, a novel strategy is applied to synthesize Fe_3O_4 NPs incorporated with sodium lignosulfonate (LS) and *N*-((1*H*-tetrazol-5-yl)carbamothioyl)benzamide (TCB) with a long tail ((3-chloropropyl)trimethoxysilane) to immobilize copper catalyst designated as MLS@TCB-Cu(II) (**Scheme 1**). The prepared catalyst was used as an efficient and magnetically recyclable catalyst for synthesizing *N*-sulfonyl-*N*-aryl tetrazoles. All the expected products were obtained in high yields, indicating the high efficiency of this catalyst for the preparation of various tetrazoles.



Scheme 1: The proposed structure of MLS@TCB-Cu(II).

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Synthesis of Magnetic Agarose Sorbent for Extraction and Preconcentration of Remdesivir

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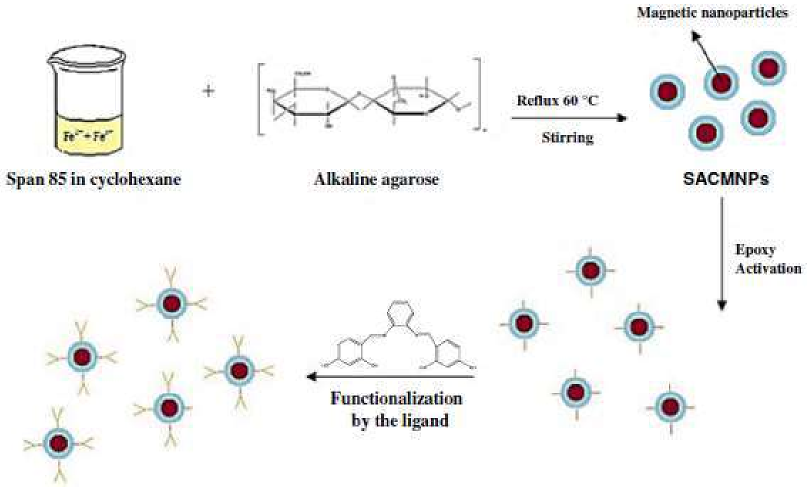
Keywords: Magnetic Agarose, Remdesivir, Extraction, Magnetic solid-phase extraction

A magnetic solid-phase extraction method based on agarose coated magnetic nanoparticles coupled to a new magnetic field agitation (MFA) device was developed and used for the preconcentration Remdesivir. The results indicate that the functionalized agarose coated magnetic nanoparticles by the ligand is efficient for the preconcentration and subsequent chromatography determination of Remdesivir. The CCD method was efficient for simultaneous optimization of the factors such as effects of pH value, ionic strength and amount of the adsorbent on the extraction and attainment of quantitative recovery for the analyte. Six replicate analyses under optimized conditions resulted in a recovery of 99.1 % with a relative standard deviation of 4.66 % for Remdesivir. The detection limit of the method (at a signal-tonoise ratio of 3σ) is 5.6 $\mu g\ L^{-1}$. samples.



Scheme1: Schematic representation of the preparation of particles and their activation and functionalization by the ligand.

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Nature of metal-ligand bond in Ni(II), Cu(II) and Zn(II) complexes of a number of tetradentate(N_2O_2) symmetric Schiff base ligands

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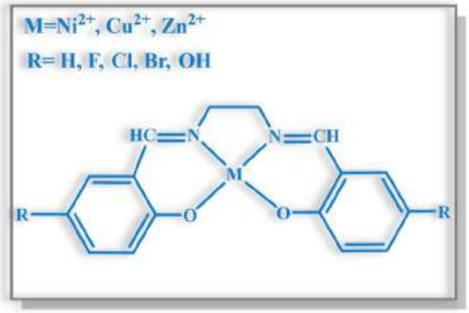
Keywords: Computatianal Study, Salen complexes, Interaction energies, nature of bond.

Schiff bases that play an important role in the development of coordination chemistry result from the reaction between primary amine with an aldehyde or a keton under specific conditions [1]. Schiff bases are the most commonly used in many domains[2]. These complex molecules are used as catalysts in many of these publications and have started to gain importance in industrial applications. In addition to these application areas, these complexes have an important place in biological activities such as antibacterial, antifungal, and antitumor, analytical chemistry, paints, polymer industries, applications of vitamins and enzymes [3]. To the best of our knowledge the nature of bond in a series of metal complexes of salen type ligands have never been studied. Herein, we want to report a theoretical study on the strength and nature of metal−ligand bond in Ni(II), Cu(II) and Zn(II) complexes of some salen derivatives (**Scheme 1**). The goemetries of all complexes were optimzed at M06L/TZ2P level of theory using ADF program. Then, the nature of bond in the mentioned complexes was studied with an Energy Decomposion Analysis of metal−ligand bond.



Scheme 1. Chemical structure of metal complexes studied here.

References

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Cooperativity of metal-ligand bonds and *trans*-influence of ligands

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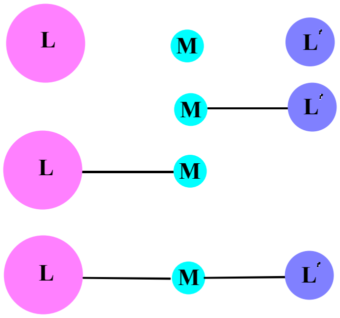
Keywords: Cooperativity, *trans*-influence, Metal complexes

Examining how chemical bonds influence one another and contribute to the overall stability of a bonded system is crucial for the rational design of targeted molecular and supramolecular structures. While there are several types of chemical bonds, extensive research over the past sixty years has primarily focused on the interplay among intermolecular noncovalent bonds, referred to as bond cooperativity.[1] Several established methodologies exist for assessing the cooperativity of noncovalent bonds and calculating the associated cooperative energies.[2] Very recently, we showed that the quantitative evaluation of the cooperative energies of all types of chemical bonds is possible.[3] Following the above studies, we want to show that the *trans*-influence of a ligand in a metal complex, defined in 1966 as the extent to which that ligand weakens the bond trans to itself in the equilibrium state of the complex,[4] can be calculated on the basis of the concept of the cooperativity of bonds (scheme 1).



L–M and M–L′ vs. L–ML′ and LM–L′

Which ones are stronger?

Scheme 1. Metal complexes formed from metal M, and ligands L and L´.

References

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Synthesis and Investigation of Toxicity and Anticancer Properties of Cycloplatinated(IV) Diacetate Complexes

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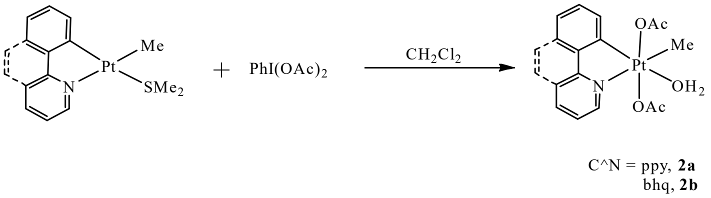
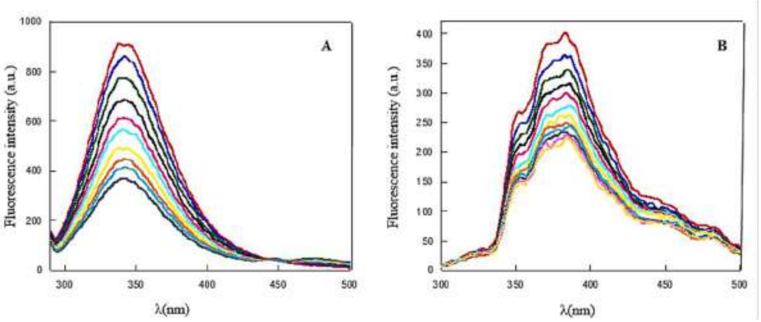
Keywords: Cycloplatinated complexes, Fluorescence, UV-Vis, Cell lines

Two cycloplatinated (IV) complexes, [Pt(C^N)Me(H_2O)($OAc)_2$] (C^N = 2-phenylpyridinate, ppy, **2a** and benzo[h]quinolate, bhq, **2b**), were synthesized from the reaction of PhI($OAc)_2$ with corresponding precursor complexes by an oxidative addition reaction (**Scheme1**). The desired complexes were completely identified using NMR spectroscopy and elemental analysis. Examining the anticancer properties of these complexes on three types of cancer cells HT-29 (human colon cancer cells), Hl-60 (adult blood cancer cells) and Raji (cancer B lymphocytes), showed that our complexes as an anticancer drug shows good performance. In the next steps, the biointeraction of platinum (IV) complexes, as antitumor agents, with bovine serum albumin (BSA) as a model of drug carrier [1] and also CT-DNA [2] were studied (**Scheme 2**).



Scheme 1: Synthesis of two complexes cycloplatinated Pt(IV) complexes.



Scheme 2: (A) Changes in fluorescence spectrum of BSA upon addition of **2a**. (B) Changes in the emission spectrum of **2b**, with increasing CT-DNA concentration.

References

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Mo (VI) Schiff base complex supported on graphene oxide and its application in the oxidation of alcohols

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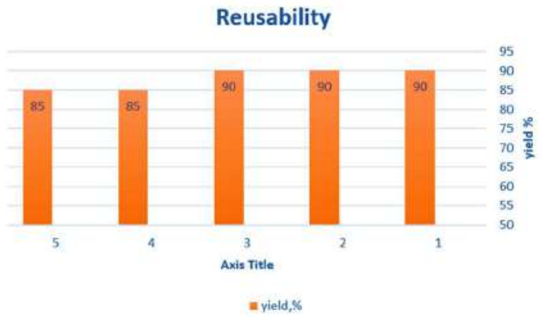
Keywords: Heterogeneous catalyst, graphene oxide, functionalized graphene oxide, molybdenum complex, alcohol oxidation

Using catalytic systems for various chemical processes has become essential in today's world [1]. Heterogeneous catalysts are particularly favored, especially for precious metals, due to their economic advantages stemming from easier recovery and separation than homogeneous catalysts. By stabilizing homogeneous complexes on suitable substrates, it is possible to synthesize heterogeneous catalysts [2]. This research used graphene oxide as a suitable substrate for synthesizing a molybdenum heterogeneous catalyst. The stabilization of molybdenum acetylacetonate complex on graphene oxide substrate functionalized by base-Schiff was investigated to oxidize alcohols. The prepared catalyst was confirmed by various methods such as FT-IR, XRD, TGA, and FE-SEM analyses. In all the reactions, the reaction conditions such as the type of solvent, the amount of catalyst, temperature, oxidant, amount of oxidant, base, and amount of base were optimized. Finally, the ability to recover and reuse the catalyst was investigated (Scheme 1).



Scheme1: Recycle of catalyst

References

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Synthesis of the Core/shell nanostructure Fe_3O_4@SiO_2@GPTMS/Schiff base-Cu(II) and its application in the organic transformation

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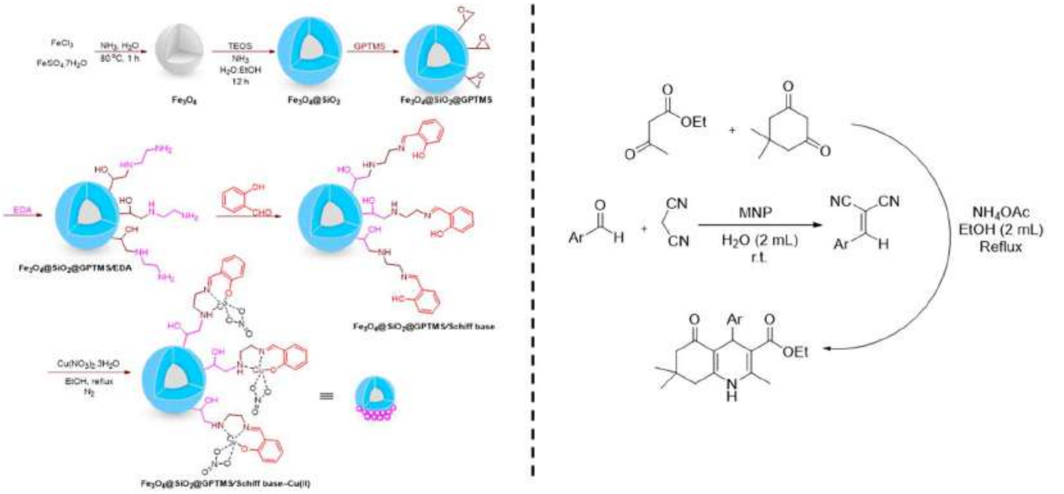
Keywords: Nano Fe_3O_4@SiO_2@GPTMS/Schiff base-Cu(II), Magnetic nanoparticles, Core/shell

The design, synthesis and development of nanoparticles (NPs) have emerged as an interesting and promising strategy. Among various types of NPs, magnetic nanoparticles e.g. Fe_3O_4 have emerged as powerful tools for the various applications in technology and industry such as drug delivery, treatment of cancer, catalysis, medical therapeutics, magnetic data storage, diagnostics, MRI, and environmental remediation [1]. Other benefits of these compounds are great dispersibility, support for immobilization of organic catalysts and metallic, high surface area, high thermal stability, and easy separation and recovery using an external magnet in reaction media. In current research, we focused on the an eco-friendly and efficient procedure for the coating of Copper(II) on the surface of Schiff base complex immobilized on Fe_3O_4@SiO_2 MNPs to synthesize a core/shell nanostructure Fe_3O_4@SiO_2@GPTMS/ Schiff base-Cu(II) nanocatalyst. Then, the as-prepared nanocatalyst was characterized various analyses such as FT-IR, FE-SEM, TEM, BET, EDX, TGA, VSM, XRD and ICP. The as-prepared nanocatalyst shows high activity in the one-pot syntheses of polyhydroquinoline derivatives of a wide range of aldehydes, dimedone, ethyl acetoacetate, and ammonium acetate and Knoevenagel condensation between aldehydes and malononitriles in good to excellent yields (Scheme 1).



Scheme 1: Preparation of Fe_3O_4@SiO_2@GPTMS/Schiff base-Cu(II) the one-pot synthesis of polyhydroquinoline derivatives and Knoevenagel condensation.

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Z-scheme $CuBi_2O_4/AgVO_3$ heterojunction for efficient visible-light photocatalytic degradation of tetracycline

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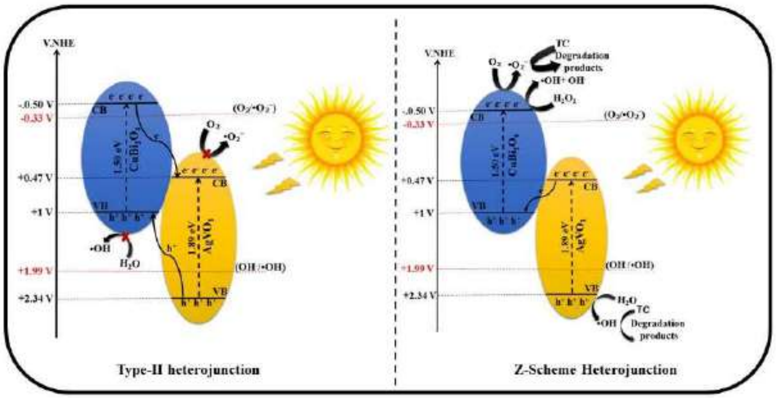
Keywords: Z-scheme heterojunction, Visible-light photocatalysis, Antibiotic degradation

The fabrication of Z-scheme heterojunction photocatalysts has emerged as a promising strategy for environmental remediation [1]. In this study, a highly efficient $CuBi_2O_4/AgVO_3$ Z-scheme photocatalyst was successfully synthesized a simple hydrothermal methods. Compared to the individual photocatalysts, the $CuBi_2O_4/AgVO_3$ heterostructure demonstrated significantly improved photocatalytic degradation capability for the removal of tetracycline hydrochloride (TCH) under visible light irradiation within 120 minutes. The optimized $CuBi_2O_4/AgVO_3$ photocatalyst exhibited the highest reaction rate constant in the degradation of tetracycline hydrochloride, which is higher than that of pristine $CuBi_2O_4$. Radical trapping experiments revealed that h^+ and $\bullet O_2^-$ were the key reactive species involved in the photocatalytic degradation process. The superior removal performance is mainly ascribed to the enhanced adsorption ability, elevated light harvesting and the increased separation efficiency originated from the synergistic effect of the components.



Scheme1: Schematic diagrams of possible charge transfer mechanism in $CuBi_2O_4/AgVO_3$.

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Comparative Analysis of UiO-66-NH$_2$ and MOF-808 in the Adsorption of Tetracycline

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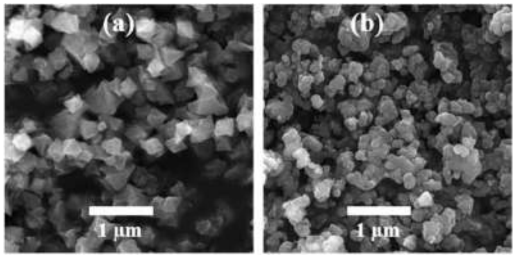
Keywords: MOF-808, UiO-66-NH$_2$, Tetracycline

This study discusses the comparison of the effectiveness of two metal-organic frameworks (MOFs), UiO-66-NH$_2$ and MOF-808, in removing tetracycline (TC) from water. TC pollution is a significant environmental concern due to its widespread use as an antibiotic, leading to contamination of water sources from pharmaceutical discharge and improper disposal [1]. The study assessed critical parameters such as adsorption capacity, BET surface area, and zeta potential to determine the suitability of these MOFs in addressing TC pollution. Experimental data was collected by exposing the two MOFs to 150 mg g^{-1} of TC solution. The adsorption capacity of MOF-808 was 275.5 mg g^{-1}, while that of UiO-66-NH$_2$ was 213.52 mg g^{-1}. The results showed that MOF-808 outperformed UiO-66-NH$_2$, demonstrating a significantly higher adsorption capacity. Referring to data in Table 1, this superior performance is likely due to MOF-808's larger BET surface area, which provides a more extensive network of pores and active sites for TC adsorption. Moreover, the zeta potential of MOF-808 (+56.5 mV) indicates electrostatic interaction, which enhances the material's effectiveness in capturing charged species like TC. In conclusion, MOF-808 demonstrates superior performance over UiO-66-NH$_2$ in adsorbing TC, as evidenced by its higher adsorption capacity, larger BET surface area, and favourable zeta potential. These findings not only suggest the suitability of MOF-808 for addressing TC pollution in water but also highlight the need for further studies to investigate the adsorption mechanisms, long-term stability, and regeneration capabilities of both materials in engineered systems. SEM images of both MOF-808 and UiO-66-NH$_2$ are also demonstrated in scheme 1.

Table 1. MOFs characteristics

MOF	BET surface area (m^2g^{-1})	Zeta potential (mV)
MOF-808	1063	+56.5
UiO-66-NH$_2$	693	+7.8



Scheme1: SEM images of (a) MOF-808 and (b) UiO-66-NH$_2$.

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Synthesis of NiS nanoparticles by Schiff base 1-benzylidene thiourea

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Keywords: Nanoparticles, Schiff base, Synthesis, Photocatalyst

In recent years Nickel sulfide nanostructures were synthesized using a hydrothermal method and a thio Schiff base ligand, 1-benzylidene thiourea , as a source of sulfide ions [1].In recent years, great efforts have been invested in the synthesis of higher ordered metal sulfide nanomaterials with specific sizes, shapes, and hierarchies, since the potential to design new materials and devices in various fields [2] .In this work, nickel sulfide (NiS) nanostructures were successfully synthesized using a new source sulfur by the simple hydrothermal method [3] . the photocatalytic properties of the synthesized nanoparticles were investigated and the morphology and structure of the compound were confirmed by XRD analysis and FE-SEM imaging. (**figure1**).

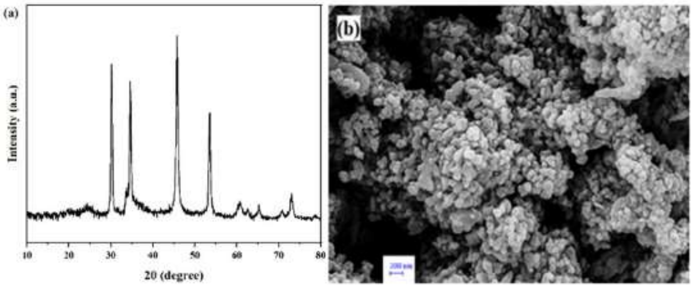

Figure 1: the synthesized NiS has a regular spherical structure with a radius of approximately 40 nm and uniform distribution.

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Using Polyacrylamide to Enhance Poor Engineering Properties of Soil

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Keywords: Polyacrylamide, Wetting-drying, Water retention

Numerous additives can be added to soils to ameliorate their poor engineering characteristics [1]. Notably, polymers are regarded as the most environmentally friendly soil additives [2]. This investigation is focused on assessing the impact of polyacrylamide on enhancing water retention and bolstering resistance to water erosion in soils. To this end, water retention tests and wetting-drying cycle experiments are conducted to ascertain these effects. In **figure 1a**, the outcomes of the water retention assessment are illustrated. The data reveals a water loss rate of 100% and 88.66% for the untreated and polyacrylamide-treated samples, respectively. Moreover, the findings demonstrate an 11.33% decrease in the water loss rate following a 24-hour period. These results can be attributed to the exceptional qualities of polyacrylamide in preserving moisture and creating a polymeric layer on the soil surface. Moreover, **figure 1b** illustrates the percentage of mass loss of a sample treated with polyacrylamide after a seven-day curing period involving wetting-drying cycles. The sample demonstrated resilience through four cycles without substantial damage and displayed remarkable resistance to water erosion due to the exceptional bonding between soil particles facilitated by polyacrylamide. In contrast, the untreated sample proved that is unable to endure even a single cycle.

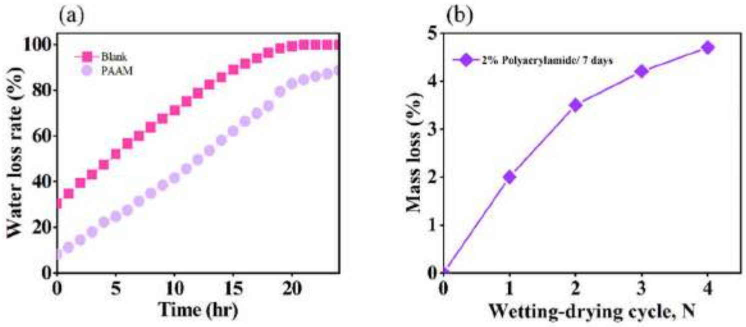

Figure 1: (a) Water retention assessment and (b) Mass loss of the treated sample

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Removal of Pb^{2+} ions by graphene oxide @ Schiff base of chitosan composite material

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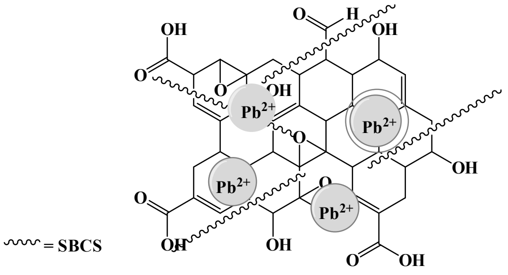
Keywords: Graphene oxide, Schiff base Chitosan, Water Treatment, removal ion.

The discharge of wastewater containing heavy metals into the environment has increased continuously as a result of various industrial activities, such as metal finishing, electroplating, metal smelting, chemical engineering, papermaking, mining, and agriculture[1]. Heavy metal contamination in such effluents presents a serious threat to the environment and human health because of their toxicity, non-biodegradability, carcinogenicity, and bioaccumulation in living organisms. For instance, lead is a common environmental pollutant present widely in manufactured batteries and also in paints and some fuels. Even in low concentrations, lead metal causes damage to the reproductive and central nervous systems in living organisms. Adsorption is the preferred technology because of its simplicity, effectiveness, and low cost in the removal of toxic heavy metals from water/ wastewater[2]. The presence of a wide range of consecutive oxygen functional groups on the GO surface and large surface area makes GO as an excellent adsorbent for the removal of heavy metals and other pollutants. CS with primary amino groups is easily functionalized with different organic ligands, such as GO, to improve its adsorption capacity. In this study, GO was fabricated with Schiff base of chitosan (SBCS) for lead removal, where GO@SBCS composite was not dispersible in water and could be easily separated by filtration or low speed centrifugation (**Scheme1**).



GO@SBCS@Pb^{2+}

Scheme1: Schematic absorption of Pb^{2+} ions by GO@SBCS

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Synthesis and Investigation of the Photocatalytic Properties of the LDH/MOF based Composite

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Keywords: Carbon nitride, Nanoparticles, Photocatalyst, Hydrothermal

In this study, we synthesized a C_3N_5/NiFe LDH/UiO-66 composite via a hydrothermal method. The structural and morphological properties of the synthesized nanocomposite were characterized using XRD, SEM, TEM, FT-IR, and UV-Vis techniques. Rhodamine B (Rh-B) was employed as a model pollutant to evaluate the photocatalytic performance of the composite under visible light irradiation. The results revealed that the C_3N_5/NiFe LDH/UiO-66 composite exhibited excellent photocatalytic activity towards Rh-B degradation. Approximately 95% of Rh-B was degraded within 75 minutes. The enhanced photocatalytic performance can be attributed to the increased specific surface area, reduced band gap, improved charge separation and transfer, and the generation of hydroxyl and superoxide radicals [1, 2]. The possible photocatalytic mechanism for Rh-B degradation was also discussed. The results of this study demonstrate that the C_3N_5/NiFe LDH/UIO-66 composite can be utilized as an efficient photocatalyst for the remediation of organic pollutants in wastewater.

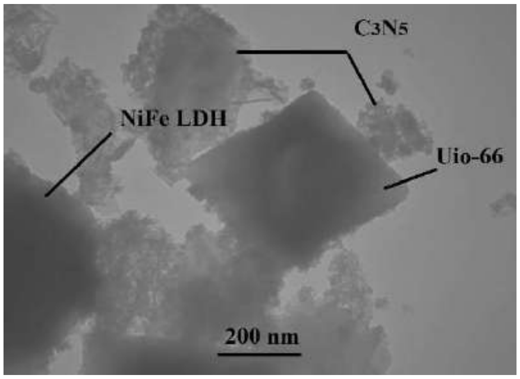

Fig.1. TEM image of C_3N_5/NiFe LDH/UIO-66.

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Electrocatalytic Degradation of Organic Dyes Methylene Blue (MB) and Congo Red (CR) in Aqueous Solutions Using Metal-Organic Nanoporous Frameworks MIL-101

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Keywords: Metal-Organic Framework (MOF), Electrocatalytic Degradation, Methylene Blue (MB), MIL-101

Methylene Blue can cause toxicity in living tissues at high concentrations and may have mutagenic effects. Congo Red, being a known carcinogen, poses health risks upon prolonged exposure. Both dyes are non-biodegradable, leading to environmental concerns due to water pollution. Additionally, they may interfere with certain biological assays by binding to proteins or nucleic acids nonspecifically [1,2]. This study investigates the feasibility of employing metal-organic framework (MOF) MIL-101 to degrade the organic dyes Methylene Blue (MB) and Congo Red (CR) in the presence of sodium borohydride in an aqueous environment at room temperature, using an electrocatalytic approach. The influence of key factors, including catalyst amount of MIL-101 and reaction time, on the degradation efficiency of the dyes at fixed concentrations was systematically examined. Dye concentration reduction was analyzed via UV-Vis spectroscopy [3-5]. The findings reveal that the catalyst MIL-101 exhibited greater efficiency in degrading Methylene Blue (MB) compared to Congo Red (CR), with optimal degradation of Methylene Blue achieved using 1 mg of catalyst MIL-101 within 1 second.

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Modification of Gum Arabic with citric acid to prepare 5-HMF

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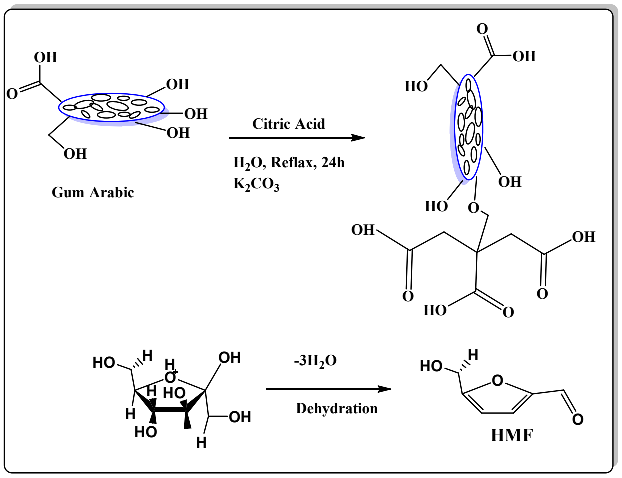
Keywords: 5-Hydroxymethylfurfural, Heterogeneous catalyst, Gum Arabic

Gum Arabic, as a heterogeneous catalyst for the conversion of fructose to 5-hydroxymethylfurfural (5-HMF) as the primary product alongside byproducts [1]. RSM was employed to optimize conditions [2], determining 43% HMF production at 110°C for 40 minutes using a 20% catalyst loading by mass. Concurrently, 57% byproducts were formed. Catalyst structural and chemical characteristics were analyses using (FT-IR), (X-ray), (SEM), and mapping. GC and GC/mass determined final product percentages (**Scheme1**).



Scheme1: The synthesis of the catalyst.

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Synthesis of modified UiO-66 metal-organic framework and its application as sensor in the detection of some antibiotics

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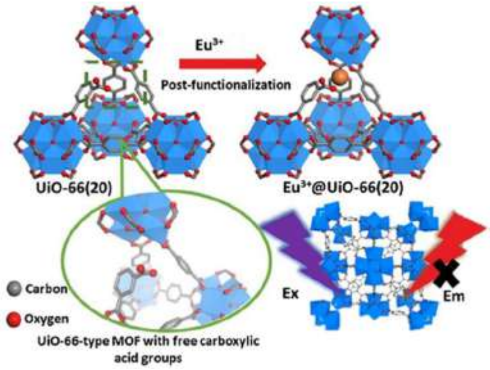
Keywords: Metal organic frameworks, UiO-66, Sensor, Antibiotic

The necessity of identifying and tracking antibiotics in biological contexts is of paramount importance. More recently, there has been a focus on the significance of identifying and tracking antibiotics in biological environments, particularly ofloxacin, to avoid environmental contamination and reduce associated risks. This issue has led to more thorough investigation into how scientists can accurately identify antibiotics. Ofloxacin can be found via chemical sensors, such as luminous sensors [1]. The use of metal-organic frameworks (MOFs), specifically UiO-66, has garnered attention due to their exceptional properties, which include their high surface-to-volume ratio, empty spaces between pores, thermal and chemical stability, and capacity for charge transfer through covalent bonds between metal and ligand. Lanthanide-doped MOFs are promising candidates for the detection of ofloxacin because of these properties. Although there are a number of methods for creating MOFs, microwave synthesis is recognized as the best method due to its faster synthesis timeframes, improved crystallinity, and higher thermal stability [2].



Scheme1: Eu^{3+} post-functionalized UiO-66-type metal-organic framework as sensor [3].

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Stability enhancement of perovskite solar cells using a multifunctional inorganic material with UV protective, self cleaning, and high wear resistance properties

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Keywords: Perovskite solar cells, ZnO, UV protective, Self-cleaning, High wear-resistance

Organometal halide perovskite solar cells have reached a high power conversion efficiency of up to 25.8% but suffered from poor long-term stability against environmental factors such as ultraviolet irradiation and humidity of the environment [1-4]. Herein, a multifunctional transparent coating containing ZnO porous UV light absorber was employed on the front of the PSCs. This strategy is designed to improve the long-term stability of PSCs against UV irradiation. Moreover, the provided coatings exhibit two additional roles, including self-cleaning and high wear resistance. The photo catalytic self-cleaning properties of these prepared coatings make them stable against environmental pollutants. Furthermore, appropriate mechanical properties such as high hardness and low coefficient of friction that leads to high resistance against wear are other features of these coatings. The devices with ZnO/Glass/FTO/mesoTiO2/Perovskite/spiro/Au confgurations maintained 30% of their initial performance for 100 h during 11 days (9 h per day) against the UV light with the high intensity of 50 mW cm-2 which is due to high absorption ZnO in the ultraviolet region. Since ZnO has a high light transmission in the visible region, perovskite solar cells with ZnO protective layers have high efficiency. It is worth noting that the mentioned features make these coatings usable for cover glass in all types of solar cells.

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Boosting and convenient production of NH_3 by using PCN-222 (Fe)/g-C_3N_4 composite through N_2 fixation process under visible light

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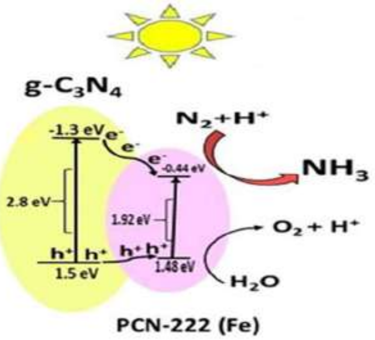
Keywords: Composite, PCN-222(Fe)/g-C_3N_4, Visible-light-driven, Metal-organic framework, Nitrogen fixation

Photocatalytic nitrogen fixation is one of the eco-friendly methods to produce ammonia gas. In photocatalytic fixation of nitrogen, transition metal atoms (ions) have the ability to chemically absorb nitrogen molecules, thereby weakening the very strong N_2 bond [1]. Zirconium-metalloporphyrin (PCN-222) facilities the fabrication of g-C_3N_4/MOFs heterogeneous junctions, overcoming challenges in photocatalytic activity. Based on existing properties, including stronger visible light absorption ability due to metalloporphyrin incorporation, increased quantum efficiency, and the chemical stability of this composite indicates that it is most likely suitable for ammonia production [2,3] (**Scheme1**).



Scheme1: Proposed mechanism of photocatalytic N_2 fixation of PCN-222 (Fe)/ g-C_3N_4 Composite.

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Synthesis and Characterization of nHA/ MgO/ GO for biological applications

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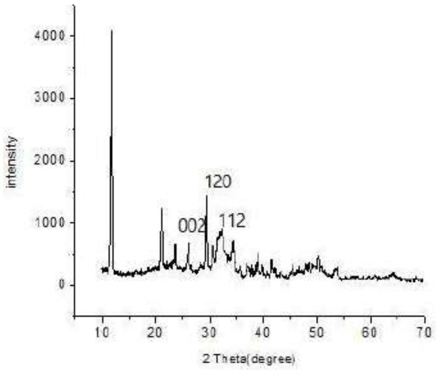
Keywords: Hydroxyapatite, Metal Oxide, MTT Assay

Nano Hydroxyapatite (nHA) [Ca10(PO4)6OH10] is a excellent selection for different applications because of its similarity of synthesis to mineral phase of the bone, excellent biocompatibility, ability to promote cellular functions, expression and osteoconductivity nHA composites were prepared and doped with graphene Oxide (GO), MgO , using the chemical precipitation method. synthesized samples were identified by the Fourier transform infared (FTIR), Field emission scanning electron microscope (FESEM), X-ray diffraction (XRD) . Phase analysis of the prepared powders was conducted using XRD. This pattern reveals that all reflection peaks of each sample still corresponded to the nHA phase, and that no other phase could be detected. FESEM results showed that nHA and nHA/GO composite displayed rod-like and spherical shapes, respectively. The results of the cytotoxicity assay revealed an acceptable limit for the cell growth and proliferation (**Scheme1**).



Scheme1: XRD pattern of nanocomposite(nHA /MgO/GO).

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The synthetic strategies of COFs, for drug delivery, photo/sono-dynamic, photo/microwave thermal and combined therapy

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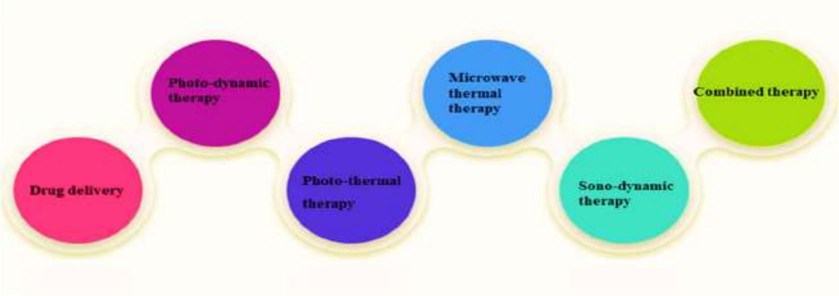
Keywords: Synthesis of COFs, Photothermal therapy, Sonodynamic therapy, Photodynamic therapy, Drug delivery

In recent years, there is an urgent need to discover synthesized anticancer drugs against drug resistance and tumor recurrence. Covalent Organic Frameworks (COFs) with different chemical constituents and functionalities have been attracted as a kind of crystalline porous polymeric materials for simultaneous cancer diagnosis and therapy purposes. The structural diversity and complexity of COFs were synthesized by various linkers including B–O covalent, imine, hydrazone, Schiff Base, triazine, azine, and β-KetoEnol. Synthesis strategies for preparing COFs including nanoparticles, thin films, and powder was introduced. COFs obtained from powder synthesis were prepared by thermoelectric, negative ion, microwave and sonochemical methods. COFs were utilized for drug delivery, photodynamic therapy (PDT), photothermal therapy (PTT), microwave thermal therapy, sonodynamic therapy, and combined therapy and combination remedy.



Scheme1: Applications of COFs.

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High surface area mesoporous sorbent composite for efficient eliminating of uranium (VI)

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Keywords: $TiO_2@Fe_3O_4$, High surface area, Uranium (VI)

The first step of adsorption studies is focused on developing a suitable, accessible, reusable, and cost-effective adsorbent for target species [1]. Kinetic of adsorption should be fast to shorten recovery time, particularly when eliminating hazardous radio nucleids, as it is important to reduce operator exposuring time. In this research $TiO_2@Fe_3O_4$ nanocomposite sorbent was synthesised and applied as a fast and effiecient adsorbent for uptake of UO_2^{2+} ions from waste. The pore diameter and surface area of $TiO_2@Fe_3O_4$ were measured at 2.5 nm and 131.8 m²/g, respectively and magnetic properties of $TiO_2@Fe_3O_4$ makes the task of separating these fine nanomaterials from the solution be facilated. Moreover, based on its psedo second order and kinetics thermodynamic data, it is aknowledged that the sorption mechanism is chemical adsorption.

The adsorption of Uranium (VI) on $TiO_2@Fe_3O_4$ sorbents was studied at various pH levels, and the impact of contact time on the distribution coefficient of uranium (VI) adsorption was investigated. (**Figure1**).

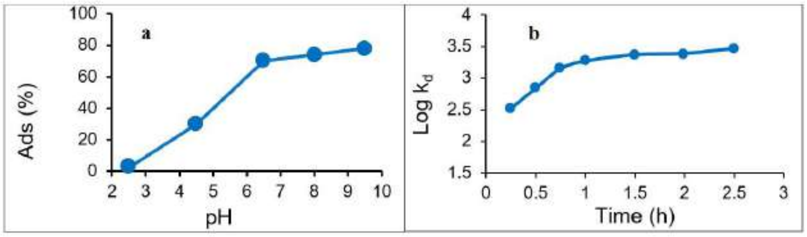

Figure1: Adsorption of uranium (VI) onto TiO2@Fe3O4 sorbents under varying pH levels (a) and the impact of contact time on distribution coefficient of uranium (VI) adsorption (b)

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Synthesis and Characterization of Hybrid Structures derived from Pyrolyzed-Metal Organic Frameworks

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Keywords: Metal Organic Framework, MOFs-derivative, Photocatalytic degradation

Photocatalytic technology is used as a method to remove pharmaceutical pollutants in water due to its low energy consumption, environmental compatibility, and high efficiency.

The pyrolysis of organometallic frameworks leads to the formation of metal oxides with large specific surface area and available active sites, thereby increasing photocatalytic properties. (**Scheme1**).

Scheme1: ZIF-67 Derived Hollow Structured Co3O4 Nanocatalysts.

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Synthesis, identification and application of nanocomposite Ag_2O, MoO_3 and Cr_2O_3 on reduced graphene oxide in order to remove dyes and organic pollutants

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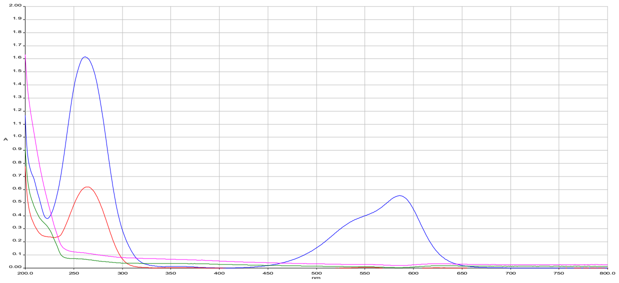
Keywords: Nano metal oxide, Nanocomposite, Reduced graphene oxide, Azo dyes, Oxidation

In this research, a mixture of silver, molybdenum and chromium oxides with two chemical ratios of 1:1:1 and 2:2:1 was synthesized by coprecipitation method and then the synthesized catalyst was stabilized on the reduced graphene oxide substrate. The synthesized nanocomposite was identified using (FTIR), Raman spectroscopy, (SEM), (EDS), XRD) methods.[1] The application of the synthesized nanocomposite was investigated in the two areas of removing azo dyes and oxidation of some organic compounds. The first part of the investigation of the use of this compound as an adsorbent for the removal of methylene blue and methyl violet dyes was investigated, and under optimal conditions, this adsorbent absorbed methylene blue dye with an efficiency of 92% and methyl violet with an efficiency of 96%.[2] In the second part of this research, the performance of this nanocomposite in the oxidation of olefin and benzyl alcohol was investigated, and under optimal conditions, the oxidation of olefin with a conversion percentage of 91% and the selectivity of 35% benzaldehyde and 53% styrene epoxide as well as the oxidation of benzyl alcohol with a conversion percentage of 99% were performed.



Scheme:Absorption of methyl violet dye.

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Synthesis, Characterization and spectral properties of a new symmetric Schiff base ligand with N, S, O donor atoms and its metal complexes

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Keywords: Schiff Base, Symmetry Compound, ^{1}HNMR Spectroscopy, UV-Vis Spectroscopy

In this study 1,2-bis(2-aminophenylthio)ethane was synthesized by the reaction of 2-aminothiophenol and 1,2-dibromoethane. Then Schiff base ligand 6,6'-((1Z,1Z')-(((ethane-1,2-dibis(sulfanediyl)bis(1,2-phenylene)bis(azanylidene)bis(2,4-di-tert-butylphenol) was synthesized by the reaction of 1,2-bis(2-aminophenylthio)ethane with 3,5-ditertsalicylaldehyde. Then their relevant complexes were obtained from the reaction of Schiff base ligand with these ions; Cd(II), Cu(II), Co(II), Zn(II) and Ni(II)[1,2]. The structure of ligand and obtained complexes were identified by spectroscopy methods; UV-Vis, FT-IR, ^{1}HNMR and mass. The results of spectroscopic characterization indicated that the intraction of the ligand with metals have an additional composition with the stoichiometry 1;1.

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Synthesis and Characterization of New Complexes With Azo Ligand Derived From "(E)-5-((2-nitro phenyl) Diazenyl)-2-Hydroxy Benzaldehyde" and Amine

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Keywords: Schiff Base, Azo Compound, ^{1}HNMR Spectroscopy, X-Ray Cryctallography

In view of recent developments and increasing of cadmium, cerium, cobalt and nickel complexes with Azo-Schiff base ligands, in the research work the schiff base of Cd(II), Ce(II), Co(II) and Ni(II) have been synthesized by reaction of $Cd(OAc)_2.H_2O$, $Ce(OAc)_2.H_2O$, $Co(OAc)_2.H_2O$ and $Ni(OAc)_2.H_2O$ with ($C_{24}H_{22}N_4O_5S$) and ($C_{23}H_{20}N_4O_5S$) schiff bases[1,2]. The new products were characterized by IR and ^{1}HNMR spectroscopies. ($C_{24}H_{22}N_4O_5S$) and ($C_{23}H_{20}N_4O_5S$) schiff base ligands have been determined by X-Ray cryctallography. The spectroscopic data suggest that in these complexes the schiff base ligands are coordinated as deporton from through oxygen and nitrogen atoms with cadmium, cerium, cobalt and nickel.

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Synthesis of g-C_3N_4 magnetic based nanocomposite and investigation of its photocatalytic properties

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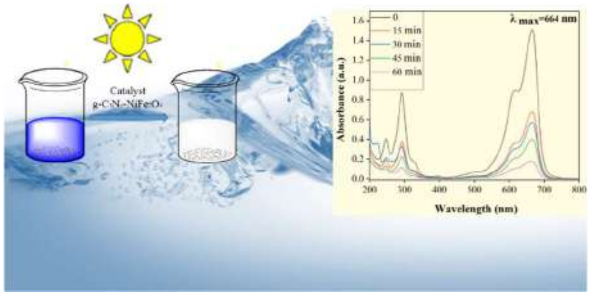
Keywords: Graphitic carbon nitride (g-C_3N_4), photocatalyst, magnetic nanocomposite, dye degradation.

With the increase of industrial activities, the pollutants entering the water systems also increase, which leads to the reduction of vital healthy water resources. This process creates serious risks for the health of the environment and humans, as well as for the ecosystem [1]. To solve these challenges, researchers are investigating innovative solutions beyond traditional water purification methods. One notable approach is photocatalytic technology, which uses light-activated catalysts to effectively degrade organic pollutants in water [2].

In this study, we synthesized a specific nanocomposite, g-C_3N_4-$NiFe_2O_4$, using a hydrothermal method. After synthesis, the nanocomposite was thoroughly characterized using XRD, FE-SEM, FT-IR, and TEM techniques. Our results indicate that g-C_3N_4-$NiFe_2O_4$ exhibits remarkable photocatalytic properties, successfully degrading over 70% of methylene blue dye within 60 minutes, highlighting its potential for water purification applications. (**Scheme1**).



Scheme1: Effect of time on dye degradation

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Synthesis and characterization of a new nanocompsite derived from "N-hydroxy succinamide" on the surface of $Fe_3O_4@SiO_2$ and investigation of its catalytic properties

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Keywords: Fe_3O_4, Nanocompsite, Catalytic properties

Application of magnetic nanoparticles as efficient supports for homogeneous catalysts has attention of researchers. Magnetic nanoparticles often contain two components, a magnetic material and a functionalized chemical component. These particles can be well dispersed in various solvents and easily separated magnetically from a medium after adsorption, eliminating such procedures as catalyst filtration and centrifugation[1]. In this study first using $FeCl_3$, $FeCl_2$ and NH_4OH solution under certion conitions nanoparticles were prepared. Then covered by TEOS and then reacts with APTES to be prepared from the amin with "N-hydroxy succinimide". Following the preparation of the Schiff base ligand the required ligand was determined by manganes acetate and the complex was investigated. In the analysis section, techniques such as SEM, EDX and VSM have been used[2]. These techniques can produce results in relation to synthetic materials that are essential for the identification of the properties of these materials. In the results section of the SEM analysis, it has been found from the papers in the images that the nanoscale component of this material, on the other hand, can be used to determine the accuracy of the existing substance in the synthesized substanceby the EDX analysis. VSM analysis was used to investigate the magnetic properties of the synthesized material due to the presence of oxide nanoparticles.

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Magnetic graphene oxide nanocomposite as anode material for lithium-ion batteries

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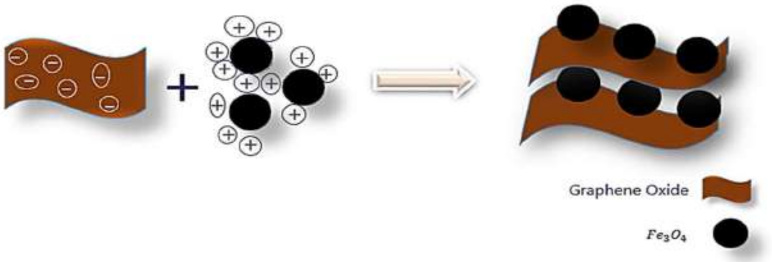
Keywords: Graphene Oxide, Magnetic, Composite, anode, Lithium Ion Battery

Today, lithium-ion batteries as energy storage devices have become the subject of constant research [1]. The performance of lithium ion batteries strongly depends on the type of electrode materials of these batteries. The use of iron oxide as anode electrode is limited due to agglomeration and large volume changes during the charge/discharge process. Making a composite of iron oxide and carbon compounds such as graphene oxide increases their performance as anodes in lithium ion batteries due to their mechanical strength and high specific surface area [2]. In this research, iron oxide with spherical morphology and average size of 100 nm was synthesized by solvothermal method and graphene oxide was synthesized by improved Hammers method. The nanocomposite derived from these two materials was synthesized by reflux at 100℃ and used as an anode. The as- prepared nanocomposite exhibited an initial capacity of 807 mAh/g, and this capacity was maintained over 20 measured cycles with 60% durability.



Scheme1: Schematic illustration of the structure of the magnetic Graphene oxide nanocomposite.

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H_2 Sensing Characterization of Pd-Doped CuO Nanoparticles; Synthesized by Solvothermal method

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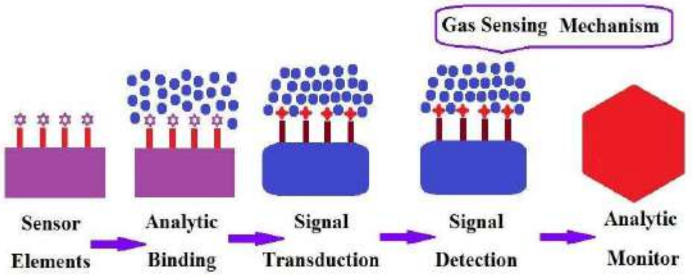
Keywords: Gas sensing, CuO, Nanoparticles, Solvothermal

Semiconductor oxides are important materials in gas-detection systems and can be improved by enhancing the sensitivity and selectivity of oxide sensors to specific gases. This research investigates the effect of palladium dopant (Pd) on the hydrogen gas-sensing ability of CuO nanoparticles. Photolithography was used to pattern electrodes on various concentrations of Pd-doped CuO thin films deposited on silicon oxide substrate, and these devices were subsequently used to measure the electrical resistance in response to hydrogen gas flow [1]. Both nanoparticles and gas-sensing characterization were conducted on the CuO thinfilm samples (Scheme1). For the nanoparticles characterization of the thin films, scanning electron microscopy (SEM) was used to determine the effect of various concentrations of dopant on the grain structure. X-Ray Photoelectron Spectroscopy (XPS) was used to verify the composition of the Pd-doped CuO thin films; X-Ray Diffraction (XRD) was used to determine the crystal structure of the doped thin films. For the gas-sensing characterization, the three key assessments used to characterize the sensitivity of CuO thin films were comparisons between CuO thin-film sensors and a commercial sensor, comparisons between CuO thin-film sensors and the exposure of the CuO thin films to UV light [2].



Scheme1: The schematic gas-sensing mechanism can be explained by five processes.

References

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[2] Alireza Aslani and Vahid Oroojpour. *Physica B*, 2011, 406, 144–149.

Supported of Zirconium Complex on Lignin -coated Magnetic Nanoparticles and its Activity in the Acetylation of Alcohols

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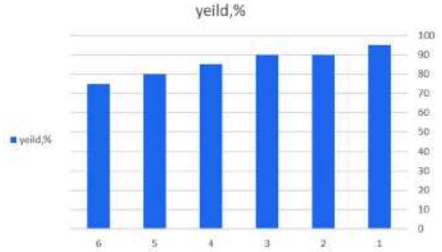
Keywords: Heterogenous catalyst, Lignin, Zirconium Complex, Acetylation of Alcohols

In heterogeneous catalysts, the active catalytic components are immobilized on an inert substrate with a large surface area, such as alumina, silica, zeolites, or various carbon structures. In the chemical industry, there is often an effort to convert homogeneous catalysts into heterogeneous ones or to incorporate nanoparticles onto porous materials. This modification facilitates the separation of the catalyst from the products and fluid reactants (whether liquid or gas). Catalytic reactions are influenced by the structure of the catalyst, its atomic arrangement, and the contact surface. These factors can be effectively controlled by adjusting the catalyst's specific composition, morphology, and size [1, 2]. In this study, the aim is to prepare a heterogeneous catalyst. Initially, iron nanoparticles are stabilized on a lignin layer. Then, using aminopropyltrimethoxy silane, the lignin structure and iron nanoparticles are aminated. A zirconium chloride complex is stabilized on the modified lignin substrate in the final stage. This catalyst is subsequently investigated in the acetylation reaction of alcohols. The synthesis steps of the catalyst were identified and confirmed using various analytical techniques such as FT-IR, XRD, TGA, SEM, CHNS, and ICP. Conditions such as solvent type, catalyst amount, and temperature were optimized in all reactions. Additionally, the effective recovery and reuse capability of the catalyst were also evaluated in this study (**Scheme**).



Scheme: Recycle of the catalyst.

References

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Offer a novel method for size appraise of NiO nanoparticles by PL analysis: Synthesis by sonochemical method

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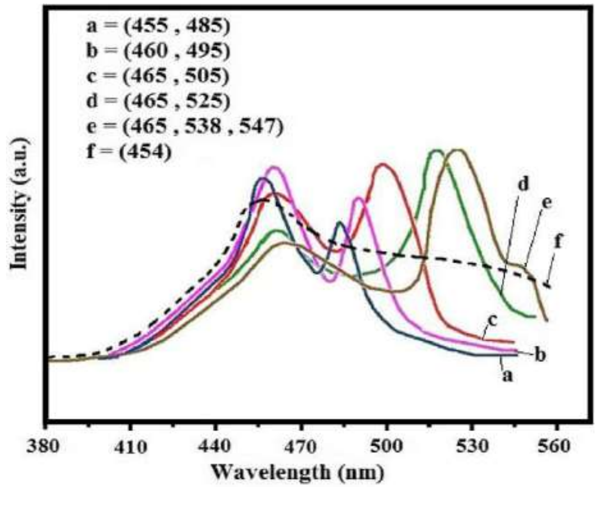
Keywords: NiO, Nanoparticles, Sonochemical

In this work, we will discuss the optical properties of NiO nanoparticles that we have investigated recently by photoluminescence (PL) spectroscopy [1]. In particular, we will show the blue-shifts of PL, originating from the electron–hole recombination of the self-trapped exciton (STE), observed in smaller-sized NiO nanoparticles [2]. To explain the size effect in relating to the STE PL shift, a question has been raised on whether it is appropriate to apply him quantum confinement (QC) theory usually used for the Mott-Winner type excitons in semiconductors to wide band-gap material, such as silica. Variations in several parameters and their effects on the structural (crystal size and morphology) properties of nanoparticles were investigated. Characterizations were carried out by X-ray diffraction (XRD), scanning electron microscopy (SEM), thermal stability (TGA and DTA), solid state UV and solid state florescent (PL) (Scheme1).



Scheme1: The solid state PL analysis of NiO nanoparticles at different size (a) 150 nm, (b) 120 nm, (c) 100 nm, (d) 60 nm, (e) 20 nm and (f) bulk size. (kex = 360 nm)

References

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[2] Alireza Aslani and Vahid Oroojpour. *Physica B*, 2011, 406, 144–149.

Preparation of PbS and PbO nanopowders from new Pb(II) coordination polymers

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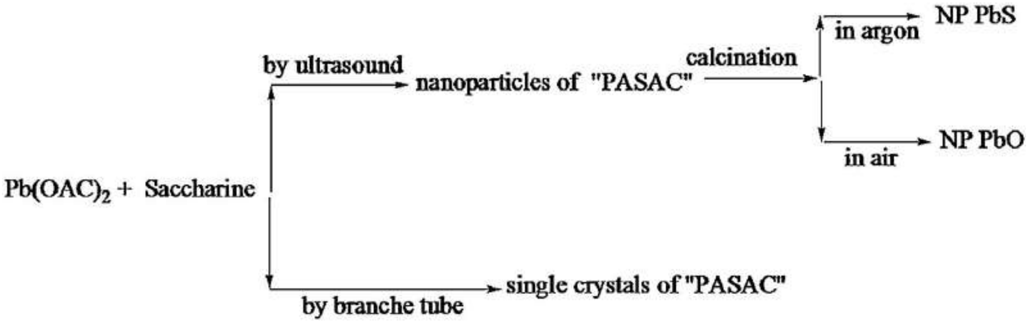
Keywords: PbS, PbO, nanopowders, coordination, polymers

Nanopowders and single crystal of new Pb(II) three-dimensional coordination polymer, $[Pb(H_2O)(OAc)(-sac)]_n$ “PASAC” were synthesized by a sonochemical and branched tube methods (Yılmaz et al., Z. Anorg. Allg. Chem. 629 (2003) 172). The new nano-structures of Pb(II) coordination polymer were characterized by X-ray crystallography analysis, scanning electron microscopy (SEM), X-ray powder diffraction (XRD), surface analysis (BET), and IR spectroscopy. The crystal structure of these compounds consists of three-dimensional polymeric units [1]. The thermal stability of compounds was studied by thermal gravimetric analysis (TGA) and differential thermal analyses (DTA) [2]. PbS and PbO nano-structures were obtained by calcinations of the nano-structures of this coordination polymer at 600$^{\circ C}$ (Scheme1).



Scheme1: Materials produced and synthetic methods

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[2] Alireza Aslani and Vahid Oroojpour. *Physica B*, 2011, 406, 144–149.

NMR parameters of a new phosphoric triamide: N-2,2-dichloroacetyl-N',N"-(bis(isobutyl)phosphoric triamide

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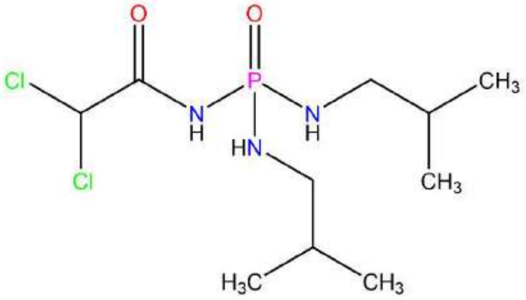
Keywords: Phosphoric triamide, Coupling constant, NMR, Spectrum.

The NMR coupling constants provide information about the different parts of a compound, leading to the assignment of signals, determination of formula[1], conformation, stereochemistry and the nature of chemical bonds[2]. Here, the synthesis of a new phosphoric triamide, $(CHCl_2C(O)NH)((CH_3)_2CHCH_2NH)_2P(O)$, is reported (Scheme 1). In the $^{13}C\{^1H\}$ NMR spectrum, the doublets at 67.32 ppm (J = 11.0 Hz) and 29.89 ppm (J = 5.6 Hz) correspond to the carbon atoms with three-bond separation from phosphorus in amide and amine moieties, respectively. In the ^1H NMR spectrum, a singlet at 9.48 ppm and a doublet of triplet at 4.51 ppm (J = 11.3 and 7.0 Hz) correspond to the NH units of the amide and amine segments, respectively. The two methyl groups of isobutyl segment appear two doublets at 0.84 ppm ($^3J_{HH}$ = 6.6 Hz) and 0.83 ppm ($^3J_{HH}$ = 6.9 Hz). Phosphorus signal in the $^{31}P\{^1H\}$ NMR spectrum is revealed as a singlet at 7.60 ppm.



Scheme 1: Chemical structure of $(CHCl_2C(O)NH)((CH_3)_2CHCH_2NH)_2P(O)$.

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A Carboxamide-Functionalized SBA-15 Probe for Selective Fe(III) Sensing

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Keywords: Fluorescence, Sensor, Mesoporous nanostructures, SBA-15, Fe^{3+} Detection

A novel mesoporous chemosensor, SBA-15@Hpiac, was developed through a post-synthesis grafting approach. This chemosensor features a silica-based SBA-15 nanostructure with fluorescent carboxamide ligand covalently bonded to its pore walls. The functionalization process involved modifying SBA-15 with (3-chloropropyl)trimethoxysilane followed by a substitution reaction with the carboxamide ligand. Characterization techniques, including FTIR, SEM, TEM and XRD, confirmed the successful attachment of the organic ligand while preserving the mesoporous structure. The fluorescence properties of SBA-15@Hpiac were investigated in the presence of various metal ions. Notably, Fe^{3+} ions induced a significant quenching of the chemosensor's emission intensity. A linear relationship between fluorescence intensity and Fe^{3+} concentration was observed Density functional theory (DFT) calculations were employed to elucidate the quenching mechanism [1-2].

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Synthesis and spectroscopic characterization of a new phosphoramide material incorporating analytical and industrial grades of melamine

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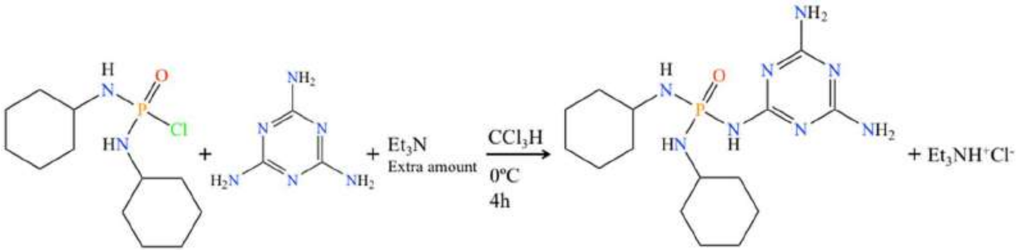
Keywords: phosphoramide, melamine, synthesis

Phosphoramides have diverse applications like in pharmaceutical and agricultural industries, and have recently gained attention for their use as fire retardants [1,2].

Melamine, a long-utilized amine in various industries, has a notable application in removing cyanuric acid from water and wastewater due to its low solubility and ability to form hydrogen bonds with this acid [3].

This research focuses on synthesis a new phosphoramide using melamine (**Scheme1**), exploring its potential for industrial production. Industrial-grade melamine was employed to compare the purity of the resulting product with that made from analytical-grade amine.



Scheme1: The reaction between melamine and a synthesized phosphorus monochloride reagent.

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Protection of power systems, AC micro grid with distributed generation sources using photovoltaics

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Keywords: Protection, Maximum power point detector, Solar cell

In this article, the main idea is taken from [1] which used the protection by the directional element in the micro grid, in the mentioned article, the size and angle of the negative sequence impedance are used to detect the direction of asymmetric faults, and the size of the current and the angle of the torque are used from the impedance. The innovation that can be considered compared to [1] is that in this article, no distributed generation source connected to the electronic power converter is considered and the method [2] is used to complete it, so our goal can be that Instead of one of the distributed generation sources in [1], a solar cell should be placed next to the inverter along with a maximum power detector (MPPT). The test system is also considered as [1], which is shown in Figure (1). In general, it can be said that the proposed method of the current research is based on the study [1] that researched on the protection of in distributed production resource units, but In the study [2], a comprehensive digital protection scheme for low voltage micro grids with inverter-based and conventional distributed generation sources is proposed. Regarding the desired innovation, we have implemented a solar cell next to the inverter along with a maximum power detector (MPPT) and replaced this set with one of the distributed generation sources (DGs (DG No. 2). We will discuss how to implement this set. Figure (2) shows the implemented innovation. As it is clear from this image, the MATLAB library was used to implement the solar cell, inverter and other circuit elements. We have tried to increase the power by sampling the current and voltage of the solar cell and using them as inputs to the MPPT control circuit. The output of the MPPT block is also given to the inverter as a control signal.

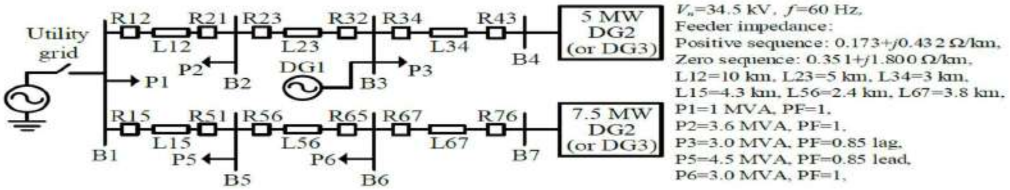

Figure 1. A layer of experimental micro grid.

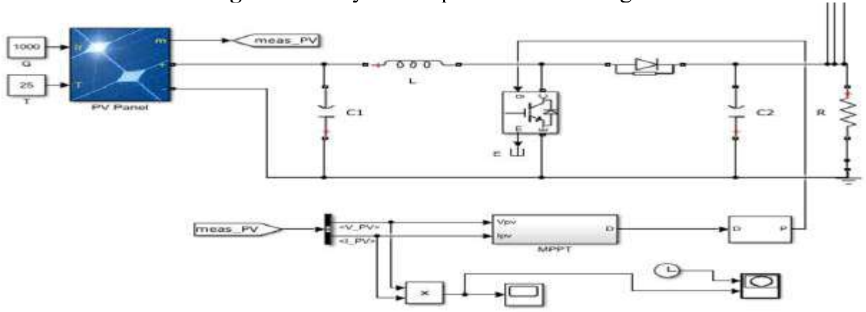

Figure (2). PV system modeling.

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Carrageenan/metal-organic framework nanocomposite: Synergistic catalytic Lewis and Brønsted acids for fructose conversion to 5-hydroxymethylfurfural

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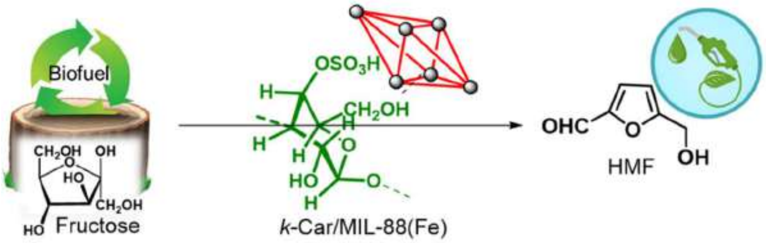
Keywords: Carrageenan, Metal-organic framework, 5-Hydroxymethylfurfural

Over the past ten years, extensive studies have focused on converting sugars derived from biomass into key platform chemicals [1]. Recently, there has been an increased emphasis on producing 5-hydroxymethylfurfural (HMF) from renewable sugars sourced from biomass [2]. In this study, a novel bio-based catalyst was developed by creating an iron (Fe)-based metal-organic framework, MIL-88(Fe), using natural sulfonic acid-functionalized polysaccharide, *k*-carrageenan (*k*-Car), (**Scheme1**). The catalytic performance of the *k*-Car/MIL-88(Fe) nanocomposite was evaluated in the acid-catalyzed transformation of fructose into HMF. Through optimization of reaction conditions, it was found that employing 40% of the catalyst at 110 °C for 30 min resulted in an impressive 98% yield of fructose conversion to HMF. With its simple production process, use of bio-based and cost-effective materials, outstanding catalytic performance, and recyclability, this green composite stands out as an environmentally friendly and efficient catalyst with significant potential applications.



Scheme1: Illustration of the fructose conversion to HMF using *k*-Car/MIL-88(Fe) catalyst.

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Theoretical investigation of chemical reactivity of the CH_3NO in the presence of MX_3 (X= Al and Ga)

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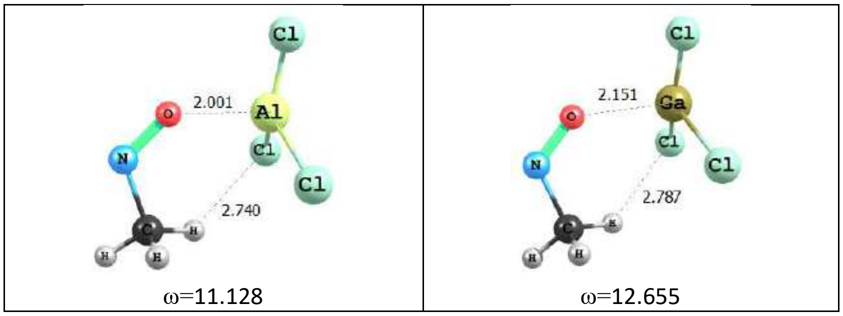
Keywords: DFT, $AlCl_3$, $GaCl_3$, Chemical reactivity, Parr functions

Density functional theory (DFT) at the M062X/TZVP level [1] have been used to examine the effect of MX_3 (X= Al and Ga) on the chemical reactivity of CH_3NO. The chemical reactivity can be obtained in terms of global and local electrophilicity (ω) through Fukui function reactivity index analysis [2]. The values of the global and local electrophilicity index are calculated for CH_3NO. The CH_3NO can be act as a dienophile in Nitroso-Diels- Alder (NDA) reactions. During the past decade, the NDA reaction has become more practical tool for organic synthesis, and numbers of important compounds have been synthesized using this method [3]. The existence of MX_3 (X= Al and Ga) has an enhancing effect on the electrophilicity and also reactivity of CH_3NO. As can be seen in schem1, the amount of global electrophilicity (ω) have been calculated for [CH_3NO…$AlCl_3$] and [CH_3NO…$GaCl_3$]. The results show that the most reactivity occurs in the presence of $AlCl_3$.



Scheme1: The optimized structures of [CH_3NO…$AlCl_3$] and [CH_3NO…$GaCl_3$] and the calculated electrophilicity.

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Synthesis and characterization of flower-like nanocomposite as a Z-scheme type photocatalyst

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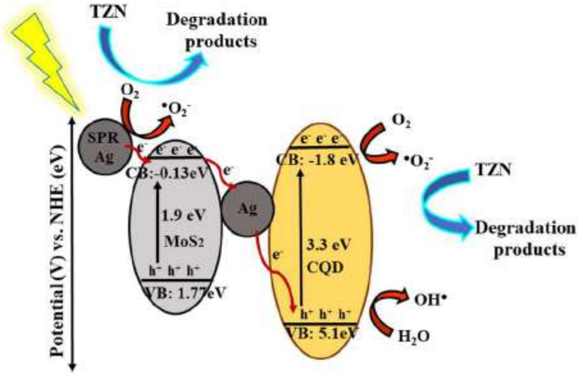
Keywords: Photocatalytic degradation, CQD, MoS_2, Dendritic Ag, Tartrazine

Nanocomposites of carbon quantum dots, molybdenum disulfide, and dendritic silver (MoS_2/CQD/dendritic Ag) were synthesized via facile and inexpensive procedure and utilized them to investigate photocatalytic degradation of tartrazine (TZN) in aqueous medium. The nanocomposites and their individual components were characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), energy dispersive spectrometry (EDS), mapping, X-ray photoelectron spectroscopy (XPS), and ultraviolet-visible diffuse reflectance spectroscopy (UV–Vis DRS). The optimum conditions for TZN degradation obtained were TZN concentration of 20 mg/L and solution pH of 6.5. Electrochemical impedance spectroscopy (EIS) and photoluminescence (PL) analysis were employed to evaluate the TZN degradation by the prepared MoS_2/CQD/dendritic Ag nanocomposites. The enhanced photo-degradation of TZN was achieved due to the synergistic effects between the nanocomposite constituents. Complete degradation of TZN occurred within 30 min with a rate constant value of 0.172 min^{-1}, wherein oxygen radicals played significant role compared to other species during the process of degradation. (**Scheme1**)



Scheme1: Schematic illustration of the possible photocatalytic reaction mechanism for MoS_2/CQD/dendritic Ag nanocomposite

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Synthesis of Bi_2S_3 nanorods using Schiff base ligand 1- benzylidene thiourea

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Keywords: Nanorods, Schiff base, Synthesis, Bismuth sulfide

In the recent years there has been a great interest for semiconductor nanomateriales in energy and environmental applications [1]. Bismuth sulfide nanorods were synthesized via a hydrothermal reaction at a relatively low temperature [2]. In this work, bismuth sulfide (Bi_2S_3) nanostructures were successfully synthesized using a new source of sulfur by the simple hydrothermal method. 1- benzylidene thiourea is used as sulfur source and capping agent simultaneously[3].The morphology and structure of the synthesized bismuth sulfide nano-rods were confirmed using FE-SEM and XRD analyses. **(Figure 1)**

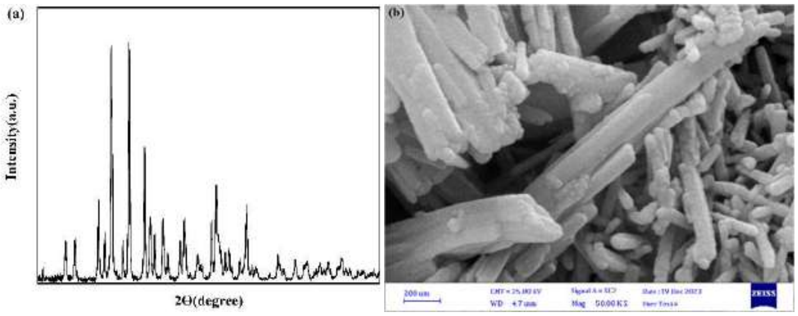

Figure 1: The synthesized Bi_2S_3 has a nanorods structure

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Immobilization of a pincer type Cu complex on the magnetic nanoparticles and its catalytic efficiency investigation

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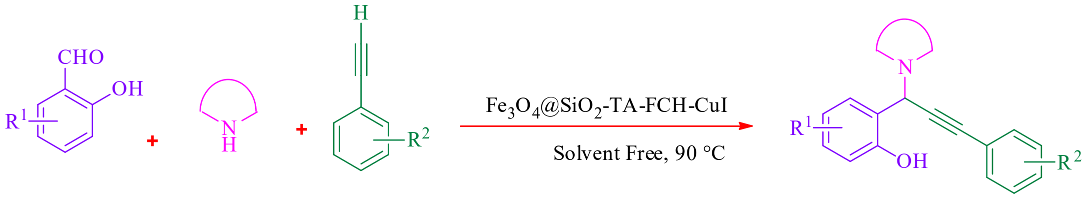
Keywords: Pincer ligand, Magnetic nanoparticles, Silica based catalyst, C-H activation

Extensive research has been done in the synthesis of pincer type complexes using organic compounds with coordinating arms such as NNN, NON, ONO, PCP and NCN. [1-2]. High thermal stability, resistance to moisture and air, low oxidation-reduction potential and excellent catalytic activity are the advantages of these types of complexes. The NCN-pincer palladium and platinum complexes were immobilized on the silica support and applied as efficient catalysts in aldol reaction [3]. *Ortho*-hydroxyphenyl propargylamines are susceptible to form orthoalkynylquinone methide intermediates, which have the capability of 1-4 Michael addition reaction with various nucleophilic active compounds. In this research, a magnetic NNN-pincer type ligand was prepared through functionalization of magnetic silica-coated nanoparticles with triazine linker agent and then furan-2-carbohydrazide compound. The catalytic efficiency of this nanocomposite after than CuI decoration on this nitrogen rich ligand was investigated in the synthesis of *ortho*-hydroxyphenyl propargylamines (**Scheme1**).



Scheme1: The magnetic NNN-pincer copper complex catalyzed the synthesis of *ortho*-hydroxyphenyl propargylamines.

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Experimental and computational studies on the binding of FAP-2286 to human serum albumin

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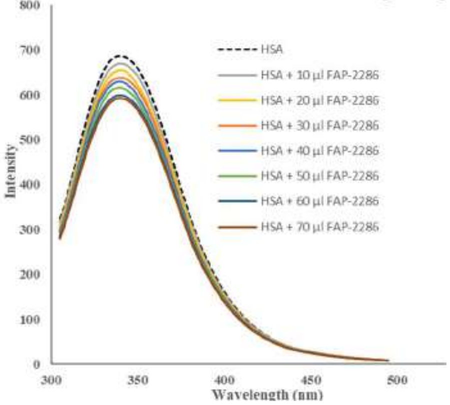
Keywords: Fluorescence, FAP-2286, Circular dichroism

Human serum albumin (HSA) is one of the major carrier proteins in the body and constitutes approximately half of the protein found in blood plasma. It plays an important role in lipid metabolism, and its ability to reversibly bind a large variety of pharmaceutical compounds makes it a crucial determinant of drug pharmacokinetics and pharmacodynamics [1-2]. In this study, FAP-2286, as well-known FAP inhibitor, were selected and prepared. The binding affinity between the above-mentioned inhibitor and human serum albumin (HSA) was studied under simulated physiological conditions (using molecular docking (MD)) and experimental analyses (using cyclic voltammetry and fluorescence spectroscopy). The obtained results revealed that the formation of a complex between HSA and FAP-2286 was responsible for quenching the native fluorescence of protein at 343 nm and can be illustrated by the static mechanism(**Scheme1**). The binding constant and number of binding sites were considered and proposed that the combination of hydrophobic and electrostatic forces were the principal intermolecular forces stabilizing the complex. The CV results demonstrate that this drug binds tightly to HSA and interact with HSA amino acids. The study provides a convenient and sensitive approach to estimate affinity parameters of the interaction between HSA and targeting compound.



Scheme1: Spectra showing the fluorescence quenching of HSA under increasing concentrations of ligand.

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Synthesis, crystal structure and Hirshfeld surface analysis of a mixed-valence iron complex

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Keywords: Mixed-valence, Ionic complex, Crystal structure, Iron complex

Iron compounds play a vital role in nature and human body. Haemoglobin is a famous example of metalloprotein that contains iron porphyrin complex [1]. Due to the ability of changing the oxidation state, iron complexes have attracted high interest in biomimetic and redox reactions [2]. They are also attractive materials in catalysis science and technology. Due to the presence of high number of unpaired electrons, iron complexes are also important compounds in magnetism [3]. Herein we report the synthesis and characterization of a new mixed-valence ion pair complex, consisting of an anionic dinuclear Fe(III) complex, $[Fe_2^{III}(\mu\text{-}O)Cl_6]^{2-}$, and mononuclear cationic complex, $[Fe^{II}(L)_3]^{2+}$ (where L = 2-acetylprydine hydrazone) and characterized by spectroscopic methods and single crystal X-ray diffraction (Scheme). X-ray analysis indicated that the Fe(II) core (in the cationic part) has distorted octahedral geometry and the N_6 coordination environment is created by coordination of nitrogen atoms of pyridine and imine functionalities of the organic ligand. The Fe(III) ions in the anionic part have distorted tetrahedral geometry and the $FeCl_3O$ around them is created by coordination of three chloride and one oxido ligands. Two Fe(III) cores are connected together by oxido bridges. The bond lengths and angles around iron ions in these complexes are close the values observed in previously reported mixed valence iron coordination compounds [4]. Due to the presence of chloride anion together with several free amine ($-NH_2$) functionalities in the structure of complex, there are several strong and directed hydrogen bond interactions in the crystal structure of this compound. Thus, Hirshfeld surface analysis was used to investigate the intra- and inter-molecular interaction in the structure of this compound.

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Biodiesel production from waste frying oil using a modified Zn coordination polymer as catalyst

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Keywords: 2D coordination polymer, Post-synthetic modification, Biodiesel

Given the pressing issues of global warming and pollution, the green synthesis and utilization of biodiesel have gained significant importance[1–3]. The present research investigates a two-dimensional zinc(II) coordination polymer, specifically modified with 1,3-propane sultone, referred to as $[Zn(AIP)(en)(PS)]_n$ (Zn-CP-en-ps), which catalyzes the transesterification of waste frying oil to generate biodiesel. In each trial, oil was placed into the reaction flask and preheated in an oil bath to the specified reaction temperature. Ethanol and the catalyst were then added, and the mixture was stirred vigorously. Upon completion of the reaction, confirmed by gas chromatography (Figure 1), the catalyst was isolated, and the mixture was allowed to settle in a separating flask for six hours. This process allowed for the separation of the biodiesel phases from the byproduct and the methanol-water mixture. The biodiesel layer was subsequently collected. The results indicated that the optimal yield of biodiesel from waste frying oil was achieved with a molar ratio of approximately 9:1 and a catalyst concentration of roughly 10% w/v.

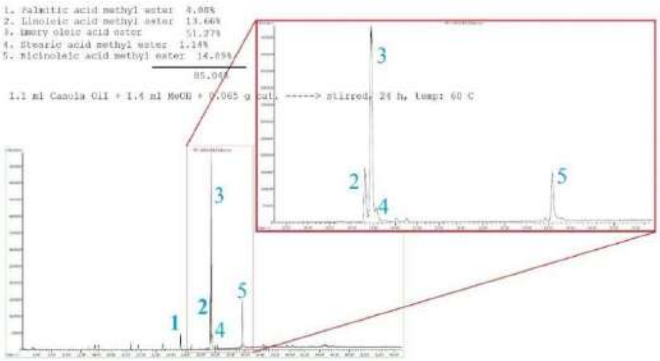

Figure 1. Gas chromatography-spectra of biodiesel sample

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Flame retardant property of synthesised $[(C_2H_5O)_2P(S)(1\text{-}NH)C_6H_4(3\text{-}NH)P(S)(OC_2H_5)_2]$: for low-density polyethylene

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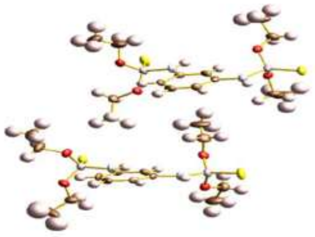
Keywords: Flame retardant, Thiophosphoramide, NMR, TGA, X-ray crystallography

Bisphosphoramidothioates have attracted attention for polymer-related applications. One of the key applications is their use as crosslinking agents to create a three-dimensional network structure [1]. This crosslinking process can enhance the mechanical properties, thermal stability, and chemical resistance. Another application of bisphosphoramidothioates is the flame retardant properties. The presence of phosphorus and sulfur atoms in these compounds can interfere the combustion process, making the polymer more resistant to fire[1].The chemical $[(C_2H_5O)_2P(S)(1\text{-}NH)C_6H_4(3\text{-}NH)P(S)(OC_2H_5)_2]$ was synthesis. The compound was characterized via FTIR, NMR (^{1}H, ^{13}C, and ^{31}P), elemental analysis, Mass spectroscopy, and X-ray crystallography. The colorless single crystals were obtained from a product solution in chloroform and n-heptane with a ratio of 1 to 4. The compound crystallizes in the orthorhombic system (Scheme 1), and space group $P2_1/n$ with a = 15.993 (3) Å, b = 16.827 (3) Å, c = 16.356 (3) Å, α = 90º, β = 110.21 (3)º, γ = 90º, V = 4130.6 (15) Å^3. The asymmetric unit consists of two complete molecules. The phosphorus signal appears at 64.61 ppm and molecular weight is 412. In the IR spectrum, the band centered at 3290 cm^{-1} is attributed to the NH stretching frequency and the P=S stretching band appears at 803 cm^{-1}. To investigate the flame retardancy, the composite sheets were prepared by adding the synthesized compound to low-density polyethylene (LDPE) using a hot press machine. Four different weight percentages of the compound were investigated (0, 0.1%, 0.3%, and 0.5%). The retardant properties of the composites were investigated by flammability, TGA, and LOI methods. The burning speeds are 26.1, 19.3, 19.1, and 21.2 mm/min for the 0%, 0.1%, 0.3%, and 0.5% samples, respectively. TGA results show that the degradation temperature for the 0% is 428.35 ºC, and for the composites, 0.1%, 0.3%, and 0.5% are 435.70 ºC, 432.05 ºC, and 435.49 ºC. LOI of 0%, 0.1%, 0.3%, and 0.5% materials are 20.7, 20.4, 21.3, and 17.9, respectively. Experiments show that the 0.3% composite has the best results.



Scheme 1: Structure of $[(OC_2H_5)_2(S)P(1\text{-}NH)C_6H_4(3\text{-}NH)P(S)(OC_2H5)_2]$.

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Synthesis and application of pillared layer mixed ligand metal-organic framework based on Zr for the synthesis of pyrazolo[3,4-*b*]pyridine-5-carbonitrile derivatives *via* a cooperative vinylogous anomeric-based oxidation

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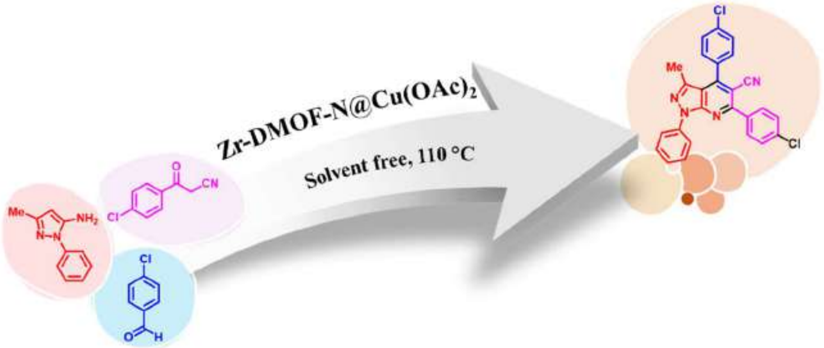
Keywords: Pillar-layered Zr-MOF, Pyrazolo[3,4-*b*]pyridine, Zr-DMOF, CVABO

Metal-Organic Frameworks (MOFs) have gained significant attention in the field of solid-state chemistry over the past two decades. These promising materials have various applications, including gas adsorption, separation, catalysis, sensing, and drug delivery. Among the research areas in crystalline materials, Pillar-layered Metal-Organic Frameworks (MOFs) stand out. Exploring their diverse structures, properties, and potential as multi donor porous frameworks is of great interest due to the numerous reports on pillar-layered MOFs. By modifying the pillar moieties along with metal nodes and oxygen donor linkers, it is possible to improve control over structure assembly and obtain structures with specific properties. The incorporation of the pyridine ring system into the structure of bioactive compounds is quite popular among *N*-heteroaromatics. This ring system is also found in natural products like nicotinic acid, nicotinamide, and vitamin B6, which play crucial roles in metabolism. (**Scheme**).



Scheme: Catalytic application strategy for preparation of Pyrazolo[3,4-*b*]pyridine derivatives using Zr-DMOF-N@Cu(OAc)$_2$

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Fabrication and Characterization of La_2MnTiO_6@Graphene Composites for Supercapacitor Electrodes

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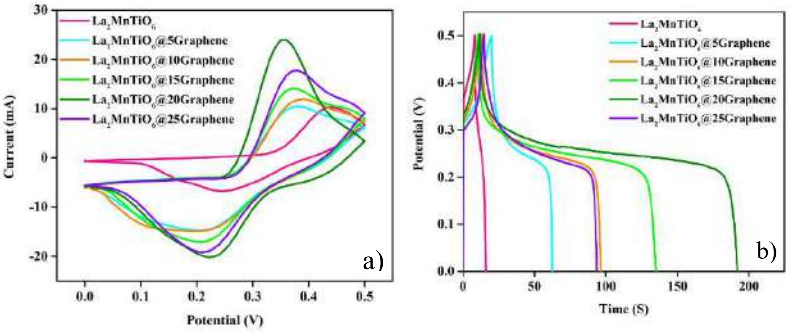
Keywords: La_2MnTiO_6, Graphene, Supercapacitor Electrodes

The growing global population and energy demand have sparked interest in renewable energy sources, particularly solar energy. However, the instability of solar power output during cloudy days and its intermittent nature make it only available on sunny days, As a result, the need for energy storage devices such as batteries, fuel cells, wind turbines, capacitors, and supercapacitors is crucial [1]. Graphene is widely used as an electrode material in supercapacitors due to its high electrical conductivity, porous structure, and stability. However, pure graphene has a low energy density due to its tendency to agglomerate [2]. Combining perovskite oxides with graphene and its derivatives has been shown to improve their electrochemical performance [3]. In this study, we successfully synthesized and characterized La_2MnTiO_6 nanocomposites with varying amounts of graphene using ultrasonic exfoliation method. The experiment we did showed that the mix with 20% graphene had the highest specific capacitance of 255.84 $F \cdot g^{-1}$ at a scan rate of 50 $mV \cdot s^{-1}$, suggesting its potential as an electrode material for supercapacitors.



Scheme1: Electrochemical performance of La_2MnTiO_6 nanocomposites with varying concentrations of graphene: (a) Cyclic Voltammetry curves and (b) Galvanostatic Charge-Discharge profiles.

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Green synthesis of MIL 101 (Cr) metal-organic frameworks using waste PET as BDC resource,

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Keywords: Terephthalic acid, BDC, Metal-organic framework, MIL 101 (Cr), Waste PET

Terephthalic acid is a large-volume commodity chemical typically produced via aerobic catalytic oxidation of para-xylene, which is produced from fossil resources. Terephthalic acid (TPA) is used primarily as a co-monomer in a condensation with mono ethylene glycol (MEG) to produce polyethylene terephthalate (PET) for plastic containers, fibers, films, and other applications. Condensations of TPA with other glycols produce other polyesters [1].
Terephthalic acid commonly abbreviated BDC. This organic compound can also be derived of waste PET bottles and is vital ingredient during the synthesis of many MOFs such as MIL-47, MIL-53, MIL-101(Cr), Uio-66, etc. MIL-101(Cr) can be synthesized both with $Cr(NO_3)_3.9H_2O$ and $CrCl_3.6H_2O$ [2]. The first experiment was carried out in a Teflon-lined Berghof high-pressure reactor containing Cr (NO3)3.9H2O and PET-derived BDC in the presence of formic acid and de-ionized water, remained at 200°C for 8h. The second method was carried out in the same condition but instead of synthesized BDC, PET flakes were used.

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Methods for synthesizing nickel salts to be used in 3D security hologram electroforming

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Keywords: Basic nickel carbonate, Nickel sulfamate, Security hologram, Electroforming

The development of the most important areas of science and technology imposes fundamentally new requirements on many inorganic substances produced by industry for the needs of the national economy. They must have predetermined physical and chemical properties and a specific physical structure. The present study provides a comprehensive method for fabricating the basic nickel carbonate particulate and nickel sulfamate electroforming solution [1]. Basic nickel carbonates were formed at a specific pH range and room temperature by the addition of nickel sulfate to sodium carbonate. The composition of the precipitates may be expressed as $NiCO_3.2Ni(OH)_2.4H_2O$ in the pH range between 7.5 to 10.0. The XRD pattern confirmed the synthesis of basic nickel carbonate and the diameter of dried particulates was less than 100 µm [2].

In the next step, as-synthesized basic nickel carbonate reacts with sulfamic acid at 50°C to produce nickel sulfamate (60% w/v). The process was optimized to achieve a clear green-colored liquid with min. 11% w/v Ni content [3]. Then an electroforming machine was designed and fabricated to produce 3D security holograms.

This system was specially designed for electroforming 3D holograms using nickel sulfamate solution without any additives. At the end of the cycle, the holograms are flexible and removed from the shims easily and immediately (**Scheme 1**).

Scheme1: Hologram production process.

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Investigating the performance of porous nanostructure Ni-Zn MOF in battery-supercapacitor hybrid energy storage system

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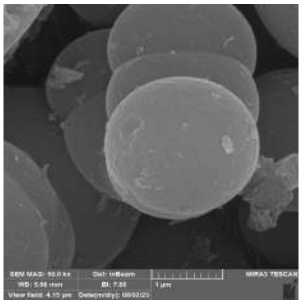
Keywords: Clean energy, Battery-supercapacitor hybrid, Metal-organic frameworks, Power density, Energy density

In this work, the design of a battery-supercapacitor hybrid storage device (BSH) is reported to achieve high power density along with high energy density. Despite the different electrochemical properties and behaviors of batteries and supercapacitors, they share similar configurations that make hybridization possible [1]. For battery and supercapacitor hybridization, we have a two-electrode cell similar to the supercapacitor system, with the difference that two asymmetric electrodes are used here [2]. So that the anode electrode is made of carbon material with supercapacitor properties and the cathode electrode is made of metal-organic framework (MOF) nanostructure based on Zn and Ni metals with battery properties to have a high energy density and compensate for the low energy density of the supercapacitor. (**Scheme1**).



Scheme1: SEM of Ni/Zn-MOF prepared by hydrothermal method.

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Investigating performance of RuNi-MOF nanosheets on nickel foam as a binder-free anode for Alanine Electrooxidation

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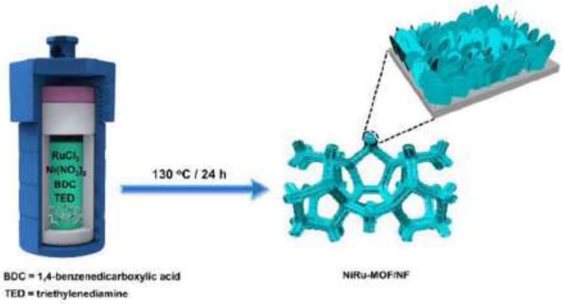
Keywords: RuNi-MOF, binder-free, electrooxidation, Nickel foam, Metal-organic frameworks

In this study, RuNi metal-organic framework was simultaneously synthesized and stabilized on nickel foam by Solvothermal synthesis method without using any binder [1]. The success of the synthesis confirmed by XRD, Raman, FT-IR, SEM, EDX and Element mapping as physical identification methods [2]. Then, electrochemical studies were performed using a three-electrode setup by CV, EIS, CA and CP techniques in alkaline conditions of 1M NaOH and 0.05M alanine. The results of electrochemical studies showed that the RuNi-MOF/NF electrocatalyst has a significant oxidation peak of 52 mA/cm^2, low charge transfer resistance of 0.5 Ohms and good stability in experimental conditions. The results of this study confirmed that RuNi-MOF/NF electrocatalyst can be used as anode in alanine fuel cell. (**Scheme1**).



Scheme1: The RuNi-MOF/NF electrocatalyst was synthesized by an autoclave with Teflon tank

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NLO response of $Ga_{12}N_{12}$ and Li@$Ga_{12}N_{12}$ nanocage: A DFT study

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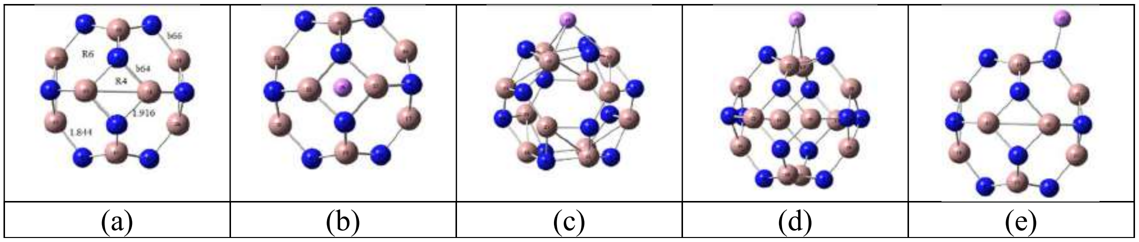
Keywords: $Ga_{12}N_{12}$ nanocage, Alkali metals, Nonlinear optical properties, Hyperpolarizability

Different types of inorganic nanocage have been reported, the most stable of which is the general formula $X_{12}Y_{12}$. The application of these nanocage in electronic devices, imaging materials, magnetic recording and environmental processes is one of the important topics in nanotechnology [1-3]. The effect of Li atom on nonlinear optical (NLO) properties of $Ga_{12}N_{12}$ nanocage has been performed using DFT calculations. All calculations were performed using the Gaussian 09 software at the B3LYP/6-31+G(d) computational level. The present computational study is performed to understand the influence of Li atom interaction with $Ga_{12}N_{12}$ nanocage on its NLO properties. (**Scheme1**).

Exohedrally adsorption of Li atom on $Ga_{12}N_{12}$ nanocage leads to significant increases in dipole moment, polarizability and remarkable NLO response. So that in the Li@fN structure, the first hyperpolarizability is significantly increased up to 4.8×10^4 au. The calculated β_0 of Li@fN > Li@R4 > Li@R6 > Li@inside structures are 47523.2 > 18418.9 > 4267.7 > 18.0 au, respectively; whereas for the pristine $Ga_{12}N_{12}$ it is 1.5 au.



(a) (b) (c) (d) (e)

Scheme1: The optimized structures: (a) $Ga_{12}N_{12}$, (b) Li@inside, (c) Li@R6, (d) Li@R4, (e) Li@fN.

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Green synthesis of 1,4- benzenedicarboxylic acid from waste PET

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Keywords: Waste PET, Recycle, Terephthalic acid, BDC

In recent decades, PETs have been widely used in the whole world. Polyethylene terephthalate is a polymer which has ester functional group in their main chain and can be both amorphous and semi crystalline. High hardness, stiffness and strength in thermoplastics, low friction and high abrasion resistance, high dimensional stability and high tracking resistance are some of the characteristics of PETs. its applications can be divided into three major categories: fiber, bottles, and industrial use [1].

Also, they can be used in manufacturing food, packaging materials, video and audio tapes and X-ray films. According to the statistics, the production of PET has reached over 24 million tons per year. Therefore, the recycle process for these polyesters is so important. Terephthalic acid commonly abbreviated BDC. Since terephthalic acid is vital ingredient during the synthesis of so many chemicals, the development of a successful process where BDC can be consistently in large quantities from waste PET for the purpose of synthesizing chemical materials would offer an economically attractive strategy for recycling waste PET. The experiment for BDC production is carried out in a Teflon-lined Berghof high-pressure reactor containing pet flakes and ethylene glycol in the presence of de-ionized water, remained at 200 °C for 8 hours [2]. The FT-IR for the commercial and the PET-derived BDC were matched.

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The effect of amine functional groups on iodine uptake capacities of a 2D Zn-MOF

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Keywords: Zn coordination polymer, Post-synthetic modification, Iodine adsorption

In this study, a two-dimensional zinc(II) coordination polymer (Zn-MOF, **1**) was chosen for consecutive post-synthetic modifications. Four different compounds were synthesized through modification of Zn-MOF on a nano scale. The first modified compound was obtained by removing of solvent molecules (DMSO) from the structure, named Zn-MOF-df **(2)**, containing open metal sites. The second and third compounds were obtained using amine molecules as Lewis base sites, namely Zn-MOF-en (**3**) and Zn-MOF-DAP (**4**), where en is ethylene diamine and DAP is 1,3-diamino propane, respectively. To invistigate the effect of different active sites on the capacity of iodine adsorption, kinetic and isotherm studies of nano-synthesized compounds were conducted in details. The results showed that the iodine uptake capacity increased from 179.51 mg/g in Zn-MOF to 498.59 in Zn-MOF-en (**3**), nearly tripling. This increase can be attributed to charge transfer transition from en as a Lewis base to the iodine as a Lewis acid[1–3]. Figure 1 illustrates the maximum adsorption capacity for the synthesized compounds.

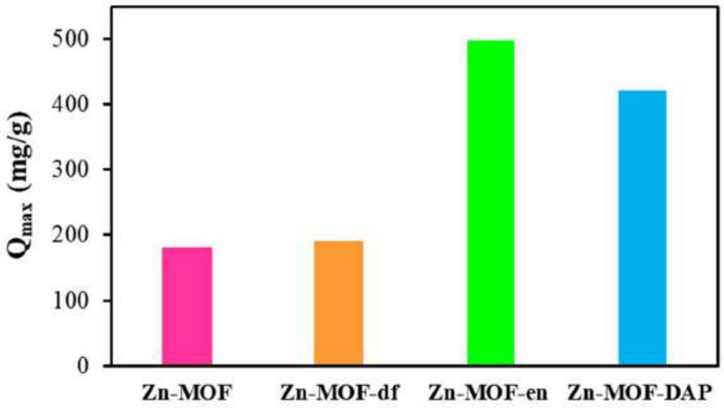

Figure 1. The iodine uptake capacity of Zn-MOF and its modified compounds.

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Synthesis, identification and characterization of composite LSPR copper nanoparticles with $NiTiO_3$ rods for photocatalytic degradation of Adriamycin

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Keywords: Photocatalyst, Adriamycin, LSPR effect, $NiTiO_3$, Copper nanoparticles

Adriamycin is one of the most common anti-cancer drugs; which is a newly emerging environmental pollutant due to genotoxicity [1]. One type of photocatalysts are titanate perovskites, represented by the general formula $ATiO_3$. In this research, we have used $NiTiO_3$ [2]. Composite of this material with copper plasmonic nanoparticles that have LSPR effect; which is cheap and abundant compared to other plasmonic metals, has improved the properties of the final order. Our composite by means of FT-IR analyzes which well shows the corresponding vibrations; Also, its band gap and absorption edge were calculated by Uv-Vis and DRS analysis, which shows 2 ev. Also, the XRD analysis showed that the patterns were completely in accordance with the reference reference code and it shows well the composite of copper with nickel titanate. Adriamycin photocatalytic degradation test shows 91.45% degradation during 120 minutes of visible light; You can see the results of the relevant analyzes in (**Figure1**).

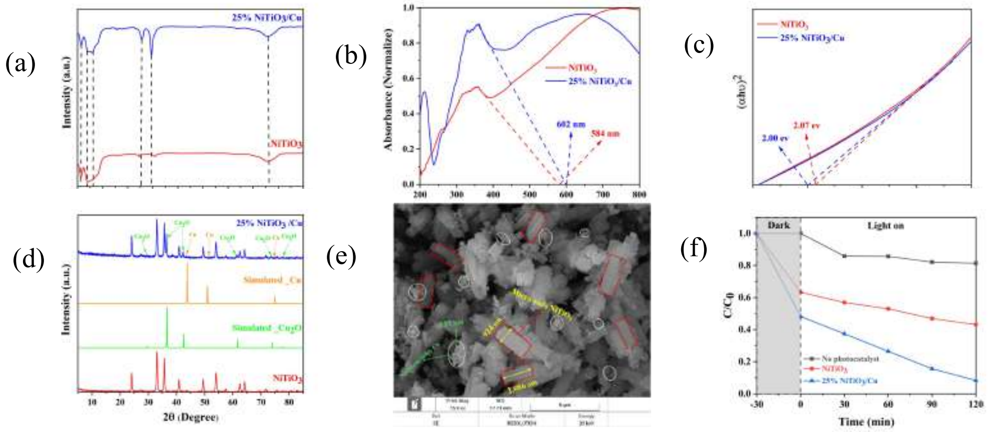

Figure1: The images you see are respectively related to the analyses (a) FT-IR, (b) Uv-Vis, (c) DRS, (d) XRD, (e) FESEM and (f) Photocatalytic degradation for $NiTiO_3$ (red color) and Composite 25% $NiTiO_3$/Cu (blue color).

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Solvent effects on the CuCl catalyzed Hetro-Diels-Alder reaction, a theoretical study

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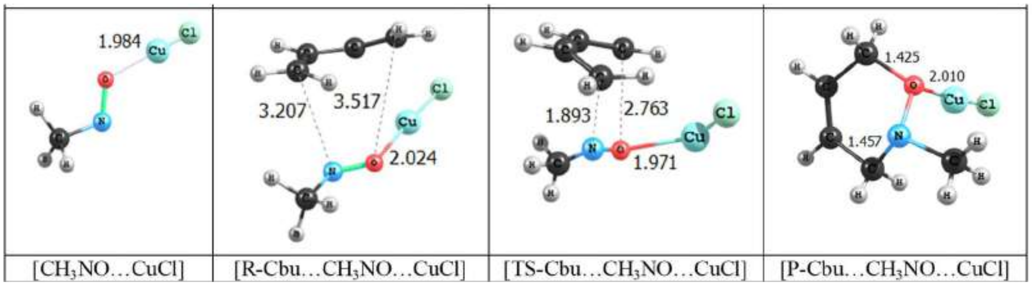
Keywords: Solvent effect, CuCl, Catalyst, DFT, Hetro Diels-Alder

In this study, the role of CuCl on Hetro-Diels-Alder cycloaddition reaction in different solvents was investigated by employing density functional theory (DFT) at the M06-2X/def2-svp level of theory using the Gaussian 09 package [1]. The copper(I)-catalyzed such as copper (I) complexes and copper salts have used Lewis acid catalyst in Diels-Alder reactions [2]. The HDA reaction is a chemical reaction for the construction of six-membered rings [3]. Some research groups investigated the effect of solvent on the rate and mechanism of different cycloaddition reactions by employing theoretical methods [4]. The aim of this work was to study the effect of solvent on catalytic effect of the CuCl in HDA cycloaddition reaction. The results showed that CuCl decrease the activation energies of NDA reaction studied here (**Scheme1**), and the largest effect occur in polar solvents.



Scheme1: The optimized structures of the catalyzed HAD reactions.

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Phosphorus chemical shifts in some new phosphoramides

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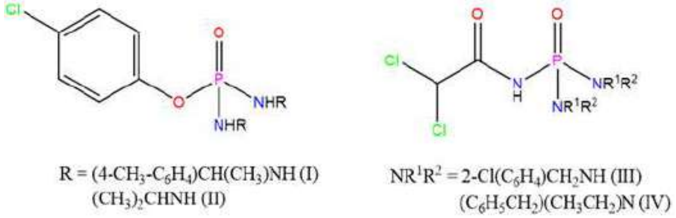
Keywords: Phosphoric triamide, Diamidophosphoester, Chemical shift, Coupling constant

Nuclear Magnetic Resonance (NMR) spectroscopy is an effective tool for identifying compounds and investigating their molecular structures. This technique provide information about the number of equivalent and non-equivalent neighbors to an atom under investigation, the types of functional groups each that nucleus is associated with, and dynamic information. Chemical shift, due to the change in the resonance frequency of the nucleus in different electronic environments, is a valuable tool for detecting changes arising from chemical reactions and geometric isomerism. Extensive databases of chemical shifts allow to predict shifts of target molecules [1,2]. In this study, several new compounds were synthesized and fully characterized using IR, ^{1}H-NMR, ^{13}C-NMR, and ^{31}P-NMR spectroscopy. The synthesized compounds are $(4\text{-Cl-}C_6H_4O)(4\text{-}CH_3\text{-}C_6H_4)CH(CH_3)NH)_2P(O)$ (I), $(4\text{-Cl-}C_6H_4O)((CH_3)_2CHNH)_2P(O)$ (II), $(CHCl_2C(O)NH)(2\text{-Cl-}C_6H_4CH_2NH)_2P(O)$ (III), and $(CHCl_2C(O)NH)((C_6H_5CH_2)(CH_3CH_2)N)_2P(O)$ (IV). The phosphorus chemical shifts in the ^{31}P-NMR spectra were investigated and compared with analogous compounds, and the effects of amine, amide and phenoxy substituents and anisotropic effect caused by arene rings were evaluated. Some topics related to IR and ^{1}H-NMR and ^{13}C-NMR spectra were detailed.



Scheme 1: Chemical structures of compounds (I), (II), (III), and (IV).

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Investigating the performance of porous nanostructure Cu-Fe MOF in battery-supercapacitor hybrid energy storage system

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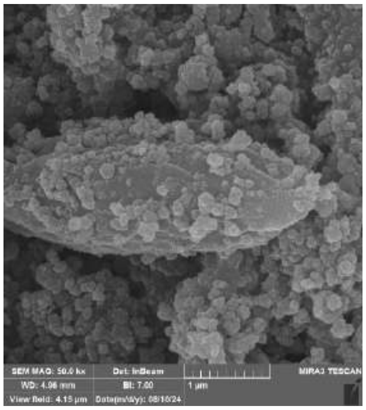
Keywords: Battery-supercapacitor hybrid, Metal-organic frameworks, Power density, Energy density

In this work, the design of a battery-supercapacitor hybrid storage device (BSH) is reported to achieve high power density along with high energy density. Despite the different electrochemical properties and behaviors of batteries and supercapacitors, they share similar configurations that make hybridization possible [1]. For battery and supercapacitor hybridization, we have a two-electrode cell similar to the supercapacitor system, with the difference that two asymmetric electrodes are used here [2]. So that the anode electrode is made of carbon material with supercapacitor properties and the cathode electrode is made of metal-organic framework (MOF) nanostructure based on Cu and Fe metals with battery properties to have a high energy density and compensate for the low energy density of the supercapacitor. (**Scheme1**).



Scheme1: SEM of Cu/Fe-MOF prepared by hydrothermal method.

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Preparation of Ni-microsphere using Ascorbic acid as coordinating ligand and study of their catalytic properties in sulfoxidation reactions and 5-substituted 1H-tetrazoles

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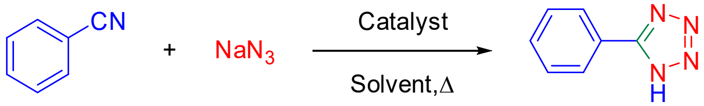
Keywords: Ascorbic acid, 5-substituted 1H-tetrazoles, Oxidation reactions, Ni microsphere

In this study, the thermal and catalytic behavior of Ni-microsphere were investigated with ascorbic acid as the coordinating ligand with different morphologie. The Ni-microsphere with ascorbic acid, as the coordinating ligand, were prepared via a solvothermal method [1]. The morphology and porosity of the obtained Ni microsphere were characterized by XRD, FTIR, TGA, EDS, WDX, AAS, DSC, BET and SEM techniques [2]. The catalytic activity of the Ni-microsphere was examined in 5-substituted 1H-tetrazoles and sulfoxidation reactions. The Ni microsphere were easily isolated from the reaction mixtures by simple filtration and then recycled five times without any reduction of catalytic efficiency (**Scheme1**).



Scheme 1. Synthesis of 5-substituted 1H-tetrazoles in the presence of Ni-Microsphere.

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Synthesis and Characterization of Copper Coordinated L-Ascorbic Acid as Coordination Polymer and its Catalytic Performance in the Organic Multicomponent Reactions

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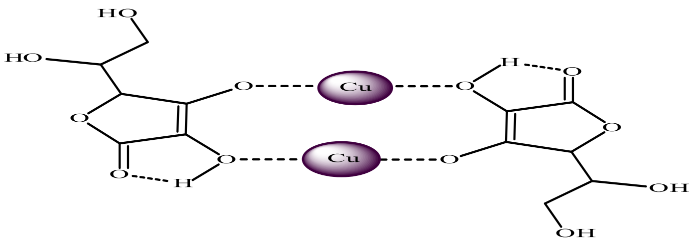
Keywords: copper, nanocatalyst, coordination, Metal-Organic Framework, L-ascorbic acid.

A copper coordinated L-ascorbic acid (Cu@AACP) Metal-Organic Framework was synthesized and characterized by TGA, FT-IR, AAS, SEM, BET, MAP and EDX. The results of the analyses confirmed the successful synthesis of Cu@accorbic acid coordination polymer (Cu@AACP) [1]. And also show any deformation of the porous structure of the parent coordination polymer. The catalytic performance was examined in synthesizing of 2, 3-dihydroquinazolin-4(1H)-ones and polyhydroquinolines [2]. The results show that an improved product yield is obtained between 84-95%. Recycle test of the catalyst confirmed that the heterogeneous catalyst exhibited good catalytic stability, efficiency and very high activity in successive runs because of its unique pore network. To show the stability of Cu@AACP nanocatalyst after recycling, the recovered catalyst was characterized by AAS, FE-SEM, EDS and FT-IR techniques (**Scheme1**).



Scheme 1: Synthesis of Cu@AACP structure.

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Green synthesis of silver – zinc oxide nanofibers by using Alcea extract

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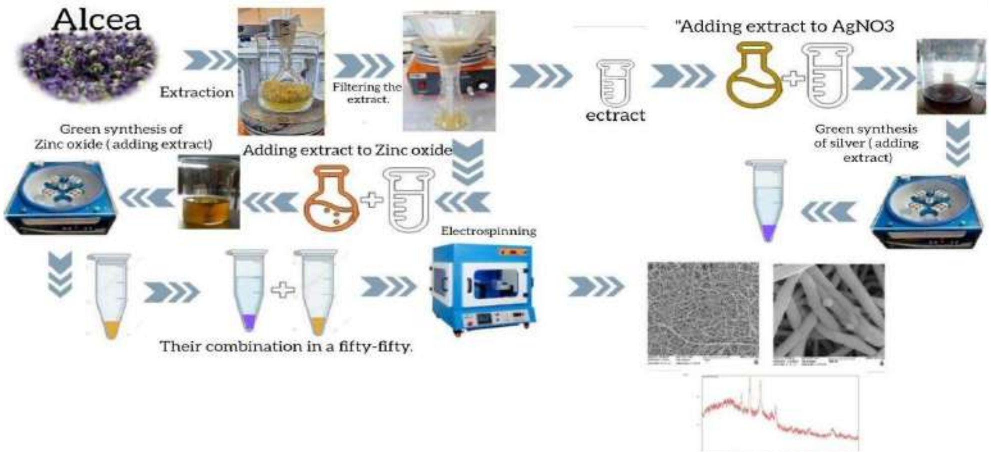
Keywords: Green synthesis**,** Nanofibers, Electrospinning, Alcea

Recent research focuses on the green synthesis of silver-zinc oxide nanofibers, highlighting their medical benefits. Utilizing Alcea, which can help alleviate pain and inflammation. The study aimed synthesize these nanofibers using hibiscus flower extract. Alcea extract was prepared through a maceration method, and the synthesis involved 2mM silver nitrate and zinc solutions. Color changes during synthesis indicated material formation. Silver-zinc oxide nanofibers were produced via electrospinning . Morphological and crystallographic properties were analysed using field emission scanning electron microscopy and X-ray diffraction, which confirmed the presence of silver and zinc oxide with specific in the XRD pattern. The images revealed that the ZnO-Ag nanofibers have a smooth and porous surface.



Scheme 1: Graphical abstract of the green synthesis process of Ag-ZnO from Alcea.

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Synthesis and crystal structure of dinuclear Mo(VI) and V(V) complexes with ONO-donor dihydrazone ligands

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Keywords: Crystal structure, Mo(VI) and V(V) complexes, Dihydrazone ligands, Synthesis

Hydrazones are a class of strong, flexible, and attractive nitrogen and oxygen donor ligands in coordination chemistry [1]. Dihydrazone ligands by having two hydrazone functional groups can form binuclear or multinuclear complexes [2]. The linker groups that connect two $-(C=O)-NH-NH_2$ units can lead to diverse structural and physical properties in these compounds. In dihydrazone ligands, the type and nature of the linker group that connects two hydrazone units can greatly influence on the structure and composition of the synthesized coordination compound [3]. Therefore, the synthesis and structural studies of new coordination compounds with dihydrazone ligands can considerably increase our knowledge about the effect of linkers in the coordination behaviour of dihydrazones. In this report, two new dinuclear Mo(VI) and V(V) complexes with general formula of $[Mo_2O_4(L)(CH_3OH)_2]$ and $[V_2O_2(L)(OCH_3)_2(CH_3OH)_2]$ have been synthesized where H_4L is a dihydrazone ligand obtained from the reaction of fumaric acid dihydrazide and 2-hydroxybenzaldehyde. Single crystal X-ray analysis indicated that both Mo(VI) and V(V) ions are six coordinated and they have MO_5N (M = Mo or V) coordination environment. The coordination geometry around metal ions in these compounds can be considered as distorted octahedral and the ONO-donor atoms of the dihydrazone ligands occupy three coordination sites. In these compounds the hydrazone ligand is coordinated to two metal ions through two ONO-donor chelating groups. The ligand has lost two phenolic and two amidic hydrogens and due to this, it can act as hexadentate ligand and provides four negative charges in the structure of these complexes. Due to the presence of coordinated methanol molecule in the structure of these compounds, there are strong intermolecular OHO hydrogen bond interactions in the crystals of these compounds which contribute in the stabilization of the crystal structures.

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Synthesis and characterization of molybdenum(VI) complex on nano-SiO_2: application nanocatalyst in oxidation of olefin epoxidation

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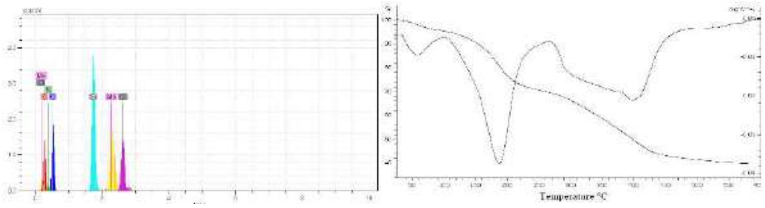
Keywords: Olefin epoxidation, Complexes of Mo, Nanoparticles

A novel organic–inorganic hybrid heterogeneous catalyst system was obtained from the reaction of the molybdenum(VI) complex and 1,4-bis(2-formylphenoxymethyl)benzene with nano-silica containing 3-aminopropyl triethoxysilane (APTS) groups. Characterization of the functionalized materials by transmission electron microscopy (TEM), scanning electron microscopy (SEM), FT-IR and thermogravimetric analysis (TGA) reveals that the molybdenum complex is successfully grafted into the pores of the host nano-silica structure. Furthermore, nanocatalyst exhibited efficient activities in epoxidation of olefins with t-BuOOH as the oxygen source. EDX analysis of the nanocatalyst showed expected elements such as oxygen, silicon, carbon, nitrogen, chlorine and molybdenum (Scheme1). The thermogravimetric analysis (TGA) curve of the nanocatalyst (Scheme1) shows the multistep mass loss of the weight between 50-600 ºC. Decomposition of the organic part is within the range of 120-600 ºC.



Scheme1: Energy-dispersive X-ray spectroscopy (EDX) (left) and TGA-DTA curve of the nanocatalyst (right)

References

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Mo(VI) complex supported on Fe_3O_4Nanoparticles: Magnetically separable nanocatalysts for selective oxidation of sulfides to sulfoxides

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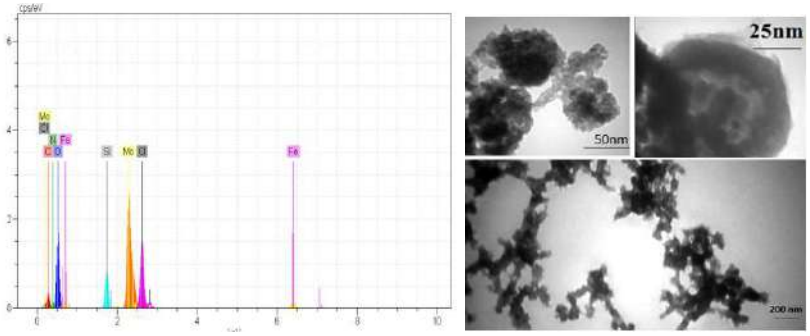
Keywords: Magnetic nanoparticles, Schiff base, Oxidation of sulfides.

A molybdenum (VI) Schiff base complex as an efficient and highly heterogeneous catalyst was developed by immobilization of a molybdenum complex on the surface of modified Fe_3O_4 magnetite nanoparticles. The obtained nanoparticles were employed as catalysts for the selective oxidation of sulfides to corresponding sulfoxides using urea hydrogen peroxide as the oxidant. Furthermore, the obtained catalysts showed not only high catalytic activity in oxidation reactions but also high degree of chemical stability in various organic solvents.

The complete characterization of catalysts was carried out by means of scanning electron microscopy (SEM), transmission electron microscopy (TEM), vibrating sample magnetometer (VSM) and FT-IR techniques. From the TEM micrographs, average particle size is estimated between 20 to 30 nm (Scheme1 right) and EDX analysis of the (Scheme1 left) showed expected elements like as iron, oxygen, silicon, carbon, nitrogen and molybdenum.



Scheme1: Energy-dispersive X-ray spectroscopy (EDX) (left) and TEM (right) images of nanocatalyst.

References

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Application of tropine-based dicationic molten salt in acceleration of synthesis of 1,2,4-triazolo[4,3-*a*]pyrimidines

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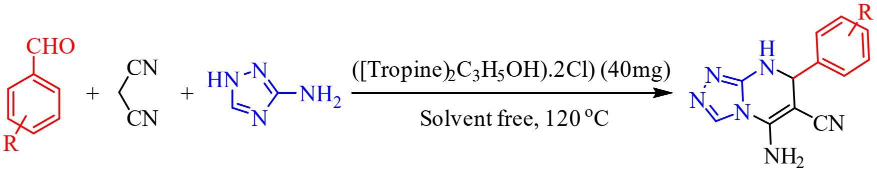
Keywords: Dicationic molten salt, pyrimidines, Tropine, [(Tropine)$_2$C$_3$H$_5$OH].2Cl

In recent years, dicationic ionic liquids (DILs) have attracted increasing interest, finding unique applications as electrolytes, catalysts and so forth [1]. DIL's characteristic caused structural variability, high tunability, low volatility, high thermal stability and lower ecotoxicity to compare with parental monocationic ionic liquids. Tropine or 3-tropanol is an important member of azabicyclo compounds which contain a tropane ring. Pyrimidine and its derivatives are important heterocyclic compounds and the diversity of their chemical and biological importance have made them more vital in pharmaceutical chemistry [2]. On the other hand, 3-amino[1,2,4]triazole derivatives which are composed of two rings, one pentamerous and the other senary, connected by a nitrogen bridge, have the ability to induce the growth of the cancer cells in the thyroid gland of rats [3]. In this work, a green and efficient procedure is reported for the synthesis of 1,2,4-triazolo[4,3-*a*]pyrimidine derivatives using a suitable dicationic molten salt based on tropine [(Tropine)$_2$C$_3$H$_5$OH].2Cl (**Scheme1**). The simple catalyst preparation, straightforward separation and recovery of the catalyst from the reaction mixture, short reaction times and high yields of the products are the significant points of interest of this study.



Scheme1: synthesis of pyrimidine derivatives in presence of [(Tropine)$_2$C$_3$H$_5$OH].2Cl.

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Application of tropine-based dicationic molten salt in acceleration of synthesis of pyrido[2,3-*d*]pyrimidine

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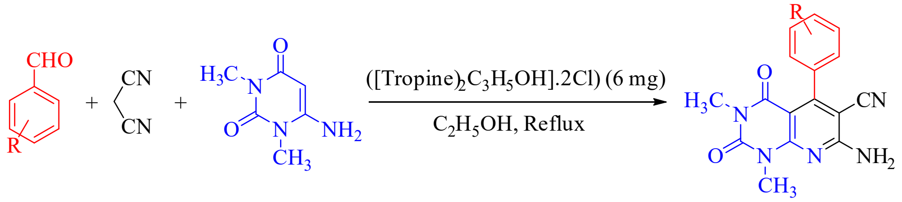
Keywords: Dicationic molten salt, pyrimidines, Tropine, [(Tropine)$_2$C$_3$H$_5$OH].2Cl

Over the past few years, dicationic ionic liquids (DILs) have garnered significant attention due to their unique applications as electrolytes and catalysts, among others. DILs exhibit structural variability, high tunability, low volatility, excellent thermal stability, and reduced ecotoxicity compared to traditional monocationic ionic liquids [1]. Tropine, or 3-tropanol, is a key compound in the azabicyclo family, featuring a tropane ring. Pyrimidine and its derivatives are essential heterocyclic compounds, and their diverse chemical and biological properties have made them crucial in pharmaceutical chemistry. Pyrido[2,3-*d*]pyrimidines possess a wide range of activities, including antibacterial, antimicrobial, tyrosine kinase inhibition, anti-inflammatory, analgesic, calcium channel antagonism, antileishmanial, and antifungal properties [2,3]. This study presents an eco-friendly and efficient method for synthesizing pyrido[2,3-d]pyrimidine derivatives using a suitable dicationic molten salt derived from tropine [(Tropine)2C3H5OH].2Cl **(Scheme1)**. The simple catalyst preparation, straightforward separation and recovery of the catalyst from the reaction mixture, short reaction times and high yields of the products are the significant points of interest of this study.



Scheme1: Synthesis of pyrimidine derivatives in presence of [(Tropine)$_2$C$_3$H$_5$OH].2Cl.

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Preparation of Ni–Fe LDH/g-C_3N_4 nanocomposite to enhance sonocatalytic degradation of tetracycline hydrochloride

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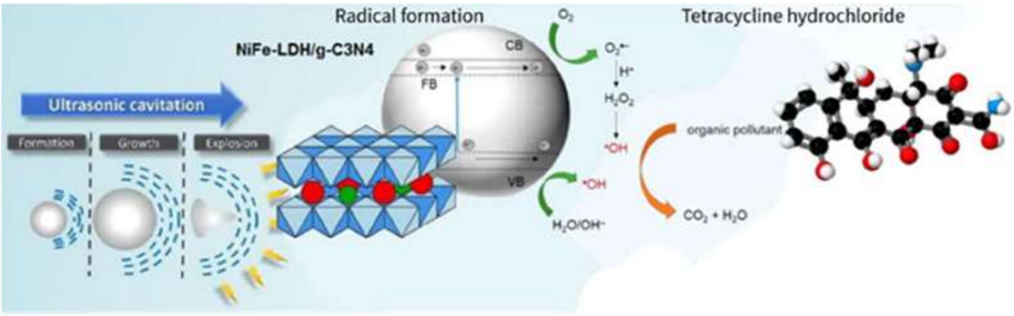
Keywords: Graphitic carbon nitride, Layered double hydroxide, Sonocatalytic degradation, Tetracycline hydrochloride.

We developed a NiFe-LDH/g-C_3N_4 nanocomposite using a hydrothermal method and tested it as a catalyst for breaking down tetracycline hydrochloride (TCH) in water [1]. They used techniques like FE-SEM, EDX, XRD, FTIR, BET, and TGA to analyze the catalyst. The optimal conditions achieved an 88.5% efficiency with 40.25 mg/L catalyst, 30.41 mg/L TCH, 349 W ultrasonic power, and pH 7.3 in 30 minutes. The proposed mechanism for TCH breakdown was detailed, and the catalyst showed consistent performance over five cycles without decline [2,3]. This study highlights the potential of this nanocomposite for water purification (**Scheme1**).



Scheme1: Mechanism of degradation of TCH.

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Preparation of Ni–Fe LDH/g-C_3N_4 nanocomposite for improved sonocatalytic degradation of chloramphenicol

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Keywords: Graphitic carbon nitride, Layered double hydroxide, Sonocatalytic degradation, Tetracycline hydrochloride

The sonocatalytic performance is defined as the increased efficacy of chemical processes via the application of ultrasonic waves, enhancing reaction rates through the generation of localized hot spots and high-energy condition The NiFe-LDH/g-C_3N_4 nanocomposite was synthesized via a hydrothermal method and tested for sonocatalytic decomposition of chloramphenicol (CAP) in water. Characterization techniques like FE-SEM, EDX, XRD, FTIR, BET, and TGA were used to analyze the sonocatalyst [1]. The study found that the nanocomposite achieved 81% efficiency in degrading CAP using 8.3 mg L^{-1} catalyst, 52.5 mg L^{-1} CAP, and 150 W ultrasonic power at pH 5 within 30 minutes. A proposed mechanism for CAP degradation was presented. The nanocomposite showed consistent performance over five cycles, indicating its potential for sustainable pollutant degradation [2,3]. Optimal efficiency was determined through experimental design, highlighting its practical application.

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A computational study of differences in phosphoramide/thiophosphoramide structures

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Keywords: phosphoramide, thiophosphoramide, crystal structure, DFT, energy framework calculations

Investigating the impact of substituent variations on molecular packing has been a topic of interest in the field of crystal engineering [1,2]. Based on the Kitaigorodskii close packing model [3], the exchanging of non-polar substituents with almost similar sizes may lead to the production of isostructures. For polar substituents, the molecular arrangement deeply depends on the electrostatic potential of the substituents [4]. In this study, a Cambridge Structural Database survey is considered to find analogous phosphoramide and thiophosphoramide structures with the three equal amine groups ($P(X)(R)_3$, X = O, S). Two pairs of similar phosphoramide/thiophosphoramide structures are found (R = $N(NH_2)(CH_3)$ (I/II) and $NHCH_2C_6H_5$ (III/IV)), and the structural analysis is carried out using the energy framework calculations to explore similarities and differences arisen from O/S exchange. The results show that the structures with smaller and more polar substituents (I/II) have completely different molecular packing maps (space groups = Pbca/$P6_3$), while in the structures with bulkier and less polar substituents (III/IV), despite the overall differences in the crystal packing maps, there are some similarities. Particularly, the strongest assemblies are similar and are constructed through NH…X=P hydrogen bonds with total interaction energies of –116.7/–100.3 kJ/mol and nearly equal electrostatic energies (–70.2/–68.5 kJ/mol). The differences in III/IV are related to the greater tendency of the P=O group to attract NH units, which makes one other assembly with a total interaction energy of –45.4 kJ/mol.

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Investigating the performance of porous nanostructure Ni-Fe MOF in battery-supercapacitor hybrid energy storage system

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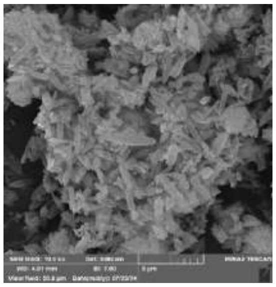
Keywords: Battery-supercapacitor hybrid, Metal-organic frameworks, Power density, Energy density

Batteries and supercapacitors are among the most widespread clean energy storage devices. In this work, the design of a battery-supercapacitor hybrid storage device (BSH) is reported to achieve high power density along with high energy density. Despite the different electrochemical properties and behaviors of batteries and supercapacitors, they share similar configurations that make hybridization possible [1]. For battery and supercapacitor hybridization, we have a two-electrode cell similar to the supercapacitor system, with the difference that two asymmetric electrodes are used here [2]. So that the anode electrode is made of carbon material with supercapacitor properties and the cathode electrode is made of metal-organic framework (MOF) nanostructure based on Ni and Fe metals with battery properties to have a high energy density and compensate for the low energy density of the supercapacitor. (**Scheme1**).



Scheme1: SEM of Cu/Fe-MOF prepared by hydrothermal method.

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Theoretical study of beryllium atom interaction with $Ga_{12}N_{12}$ nanocage

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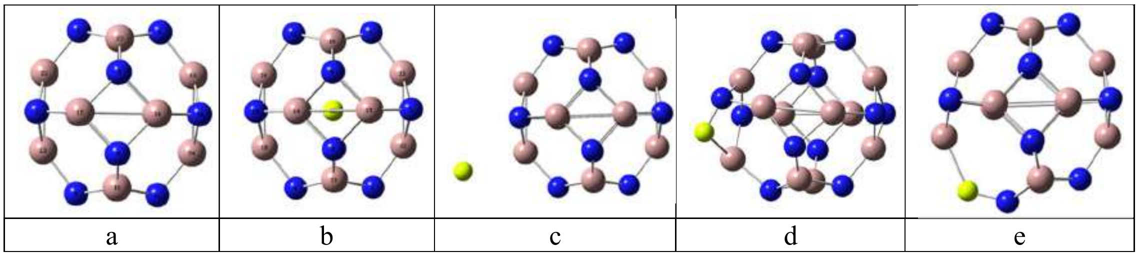
Keywords: DFT calculations, $Ga_{12}N_{12}$ nanocage, nonlinear optical, dipole moment

The impact of beryllium (Be) atom on the nonlinear optical (NLO) properties of the $Ga_{12}N_{12}$ nanocage was investigated using DFT calculations. All calculations were performed using the Gaussian 09 software at the B3LYP/6-31+G(d) computational level[1]. The results indicate that the incorporation of a Be atom leads to a substantial increase in dipole moment, polarizability, and NLO response. Specifically, the value of β0 for Be@fGa rises to 2222.1 au. The calculated β0 values for the various configurations Be@fGa, Be@R6, Be@R4, and Be@inside are 2222.1, 577.4, 572.7, and 27.2 au, respectively, compared to a value of 1.5 au for $Ga_{12}N_{12}$. Notably, the beryllium atom forms a covalent bond with the nanocage in the Be@R4 and Be@R6 positions, where it is situated within the ring structure (see Scheme 1). The adsorption energy in these positions is significantly more stable than in other locations.


a
b
c
d
e

Scheme1: The optimized structures: (a) $Ga_{12}N_{12}$, (b) Be@inside, (c) Be@R6, (d) Be@R4, (e) Be@fN.

Structures	E_{int}	RSE	E_g (eV)	μ (D)	α (au)	$β_0$ (au)
$Ga_{12}N_{12}$	-		3.020	0.005	316.7	1.5
Be@inside	-0.122	3.049	1.970	0.094	357.4	27.2
Be@fGa	-0.604	2.567	2.849	3.106	381.6	2222.1
Be@R4	-3.116	0.055	3.088	2.028	344.2	572.7
Be@R6	-3.171	0.000	3.172	2.033	341.3	577.4

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Synthesis, characterization, structural studies and Hirshfeld surface analysis of chiral copper(II) complexes

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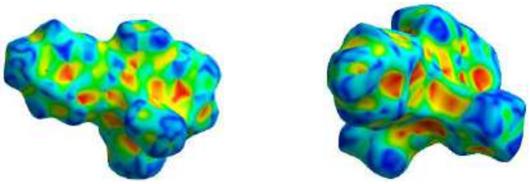
Keywords: Chiral complex, Schiff base ligands, Structural studies, Spectroscopy

The research on chirality and stereoselective synthesis of chiral molecules has attracted considerable interest in pharmacy, industry and chemical sciences [1]. The use of asymmetric synthesis in the presence of chiral catalytic systems is one of the effective methods for stereoselective and enantioselective synthesis [2]. The reaction of metal salt precursors with carefully tailored chiral ligands is an effective method for the synthesis of chiral complexes [3]. Here, we report the synthesis, characterization and crystal structure of two new chiral Cu(II) complexes with chiral ONO-donor Schiff base ligand. The chiral Schiff base ligand (H_2L) was obtained by the reaction of (R)-3-hydroxy-2-ethyl-propionichydrazide with 2-hydroxybenzaldehyde in methanol solvent and it was characterized by FT-IR, NMR and UV-Vis spectroscopic methods. Cu(II) complexes were synthesized by the reaction of $Cu(NO_3)_2 \cdot 3H_2O$ or $CuCl_2 \cdot H_2O$ with the pre-synthesized chiral Schiff base ligand in methanol solvent. The single crystals of Cu(II) complexes were achieved by thermal gradient method in acetonitrile. The obtained single crystal crystals were characterized by spectroscopic methods and their structures were determined by single crystal X-ray analysis. The Cu(II) ion in both complexes is five coordinated and has distorted square pyramidal geometry. By considering the presence of several hydrogen bond acceptor groups in the structure of complexes, intermolecular interactions were further studies by Hirshfeld surface analysis (Scheme 1) and the results confirmed the presence of intermolecular NHO, OHO and CHO interactions in the structure of these complexes.



Scheme 1. Hirshfeld surface analysis of Cu(II) complexes

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Investigating the effect of the presence of calcium carbonate on NR/SBR rubber properties

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Keywords: Calcium carbonate, NR/SBR rubber, Physical properties, Mechanical properties

Fillers are widely used in the rubber industry for many applications such as tile flooring, automotive tires, etc. Calcium carbonate ($CaCO_3$) is one of the important mineral powders that are widely used as fillers to reduce costs in the rubber industry. . The aim of this study is to investigate the physical and mechanical properties of NR/SBR rubber compound with $CaCO_3$ powder. In this study, the effect of calcium carbonate on the curing behavior of NR/SBR compound reinforced with carbon black was investigated and for the purpose of comparison, the compound with calcium carbonate and the compound without calcium carbonate were examined using sulfur curing system. The results showed that the addition of calcium carbonate causes an increase in hardness, tensile strength, and percentage increase in length and density, and on the other hand, it causes a decrease in fatigue resistance and wear resistance (**Table1**).

Table1: Formulation of compound

number	material	Phr	Phr	Weight (gr)
1	**NR (SMR 20)**	**70**	**70**	752.38
2	**SBR 1502**	**30**	**30**	322.45
3	**N550**	**50**	**50**	537.41
4	**calcium carbonate**	**0**	**35**	376.19 & 0
5	**oil**	**15**	**15**	161.22
6	**Stearic.acid**	**2**	**2**	21.50
7	**ZNO**	**4**	**4**	42.99
8	**6PPD یا IPPD**	**1**	**1**	10.75
9	**Paraffin wax**	**2**	**2**	21.50
10	**sulfur**	**2**	**2**	**21.50**
11	**CBS**	**1**	**1**	**10.75**
12	**TMTM**	**0.5**	**0.5**	**5.37**
	total	**177.5**	**212.5**	2284.00

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Synthesis of polyethylene glycol hydrogel and wastewater treatment

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Keywords: PEG, Wastewater, Hydrogel, Contaminat removal

The primary materials used in the synthesis of hydrogels consist of monomers, which can be either synthetic or natural, or polymers [1]. Hydrogels are typically prepared from polar monomers, such as hydroxyethyl methacrylate (HEMA), hydroxyethoxyethyl methacrylate (HEEMA), methoxyethyl methacrylate (MEMA), and methoxyethoxyethyl methacrylate (MEEMA) [2]. Since the first publication on hydrogels in the 1960s by Wichterle and Lim, which focused on poly(HEMA)-based hydrogels, these materials have found wide applications. One significant application of hydrogels is in the removal of contaminants from natural water sources. Polyethylene glycol (PEG)-based hydrogels are particularly advantageous for wastewater treatment, as they can effectively absorb pollutants without requiring extensive pre- or post-treatment processes [3, 4].

Scheme1: Polyethylene glycol space shape

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Synthesis and application of magnetic metal-organic frameworks as H-bond catalyst in the preparation of pyrazolo[3,4-*b*]pyridines via via a cooperative vinylogous anomeric-based oxidation

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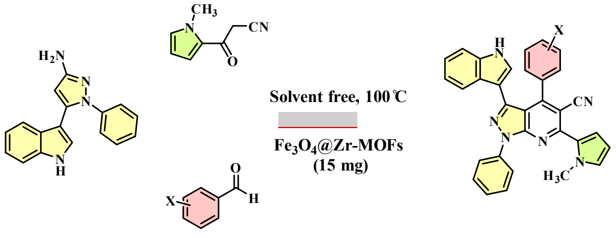
Keywords: Anomeric-based oxidation, Pyrazolo[3,4-*b*]pyridine, Fe_3O_4@Zr-MOFs, CVABO

Metal-Organic Frameworks (MOFs) are porous compounds with high design capability and controllable properties, which have been interesting research fields in recent decades. MOFs, which are also called porous coordination polymers (PCP), are obtained by covalently connecting metal clusters to organic ligands and creating a crystalline structure [1]. The broad features of MOFs, including high thermal stability, high porosity, crystalline nature, and adjustable pores, have caused these platforms ideal chemical to be used in various fields such as gas storage, targeted drug delivery, absorption, desorption, sensors, photo catalysts, and catalysts [2]. In recent years, increasing the stability of MOFs has been of great interest. An attractive perspective for this is the integration of MOFs with metallic nanoparticles (NPs). the integration of Fe_3O_4 and MOFs has been able to create compounds with interesting properties. Magnetic metal-organic frameworks (MMOFs) have wide applications in various fields such as drug delivery, catalyst, photocatalyst, separation, positioning and absorption of chemical compounds. Recent scientists pay special attention to the preparation of compounds with biological and medicinal properties. Among them, pyrazolo[3,4-*b*]pyridine are of interest with biological properties such as anti-cancer, anti-bacterial, anti-fungal and anti-parasitic.



Scheme1: Preparation of Novel pyrazolo[3,4-*b*]pyridine derivatives Using Fe_3O_4@Zr-MOFs.

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Investigating The Crystallographic Categories of Nickel Sulfide Minerals With Emphasis on Pentlandite Ore $(Ni,Fe)_9S_8$

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Keywords: Crystallographic Categories, Pentlandite, Cubic, Triclinic

Nickel minerals are found in nature in the form of sedimentary, igneous and hydrothermal deposits. Nickel is primarily present in acidic igneous rocks and is concentrated in pegmatite and hydrothermal residual solutions due to its medium ionic radius. Nickel minerals are formed as rare and complex compounds of pentlandite type and their oxidation compounds (nickeline, pyrrhotite, etc.) in pegmatites. Primary nickel minerals are found paragenetically, together with special pegmatite minerals such as beryl, muscovite, tourmaline, etc. In the magmatic environment, nickel is in the form of Ni^{2+}. Uranus ion is easily oxidized to Ni^{4+} in atmospheric water. The oxide form of nickel is transported over a wide range of pH conditions; While the reduced form of this metal is generally insoluble. Nickel can be precipitated in the form of sulfide, in the form of pentlandite, when the Eh of the fluid decreases. Nickel oxides are crystallized in cubic and triclinic crystal structure, which are crystallized in 5 crystallographic categories of cubic lattice and 2 crystallographic categories of triclinic lattice based on parameters such as temperature, pressure, time and thermodynamic fluctuations.

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Curcumin-loaded M-MOF (M = Cu, Zn)@ Polycaprolactone Nanocomposite Sponges: Fabrication, characterization, and biocompatibility assessment

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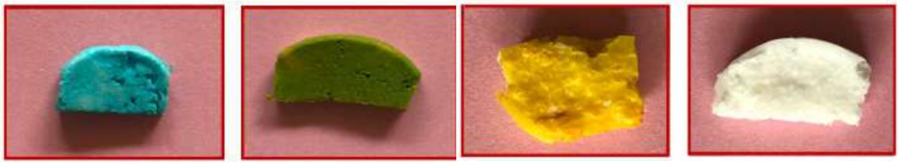
Keywords: Metal-Organic Framework; Polycaprolactone; Curcumin; Scaffold; Tissue engineering

The fabrication of multifunctional scaffolds has attracted much attention in biological fields. In this research, some novel composites of Cu(II) or Zn(II) metal-organic frameworks (M-MOFs) and polycaprolactone (PCL), M-MOF@PCL, have been fabricated as a multifunctional scaffold for application in tissue engineering (TE). The porous three-dimensional sponges were prepared by a salt leaching method. M-MOF@PCL composite sponges have been prepared by in situ synthesis of M-MOF in the presence of the as-obtained PCL sponge to gain a new compound with proper features for biological applications. Finally, curcumin was loaded into the M-MOF@PCL as a bioactive compounds that can acts as a wound healing agent, anti-oxidant, and anti-inflammatory. The presence of the M-MOF in final composites were investigated by different methods such as FTIR (Fourier-transform infrared), XRD (X-ray diffraction), SEM (scanning electron microscope), and EDS (energy dispersive X-ray spectroscopy. According to the EDS images, M-MOFs were uniformly incorporated throughout the PCL sponges. In vivo investigation on a third-degree burn model in adult male Wistar rats exhibited an accelerated wound healing for Cu-MOF@PCL compared to with Zn-MOF@PCL and the control group[1-4].



Scheme1: M-MOF (M = Cu, Zn)@ Polycaprolactone Nanocomposite Sponges.

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The effect of electrodeposition time on surface morphology and crystal structure of electrodeposited nickel nanocones

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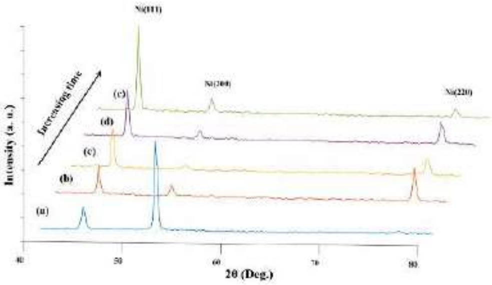
Keywords: Electrodeposition, Nickel nanocones, Crystal modifier

Electrodeposited nickel nanocones are a new class of advanced materials that have attracted attention in energy applications such as lithium-ion batteries [1], supercapacitors [2] and catalysis of hydrogen evolution reaction (HER) [3]. In this work, nickel nanocones were galvanostaticaly (J=0.45 mAcm^{-2}) electrodeposited on copper substrates from a nickel chloride (1 M) bath containing calcium chloride (1.2 M) as the crystal modifier. The effect of the electrodeposition time on surface morphology and crystal structure of the electrodeposited nanocones was investigated. According to X-ray diffraction (XRD) results, it was found that at lower electrodeposition times, the crystals grow in Ni (200) direction whereas, at high electrodeposition times the preferred orientation is Ni (111). Scanning electron microscopy (SEM) showed that the sharpest apex angle of the electrodeposited nanocones is observable at the deposition time of 10 min.



Scheme1: X-ray diffraction patterns of the nickel nanocones electrodeposited at different times of 6 (a), 8 (b), 10 (c), 12(d) and 14 (e) min

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Biosynthesis of Ag NPs/ *Mespilus germanica* kernel substrate as a green and retrievable Catalyst for Wastewater treatment

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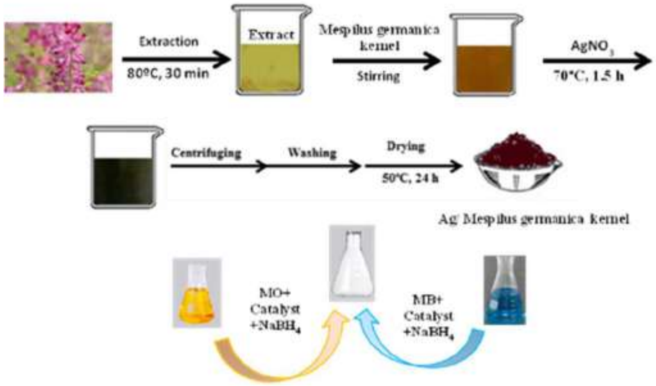
Keywords: Ag NPs/ Mespilus germanica kernel, Green synthesis, Wastewater treatment, Retrievable Catalyst

Azo dye compounds are well known as toxic, bio-refractory and carcinogenic pollutants in wastewaters so, removal of these harmful pollutants is essential. In this research, Ag NPs/ Mespilus germanica kernel as an effective catalyst was prepared through reduction of Ag^+ ions using *Fumaria officinalis* extract as the reducing and capping agent and Ag NPs immobilization on Mespilus germanica kernel surface in the absence of any stabilizer or surfactant. The as-prepared catalyst was characterized by Fourier transform infrared (FT-IR) and UV-Vis spectroscopy, field emission scanning electron microscopy (FESEM) equipped with an energy dispersive X-ray spectroscopy (EDS), Elemental mapping and, X-ray diffraction analysis (XRD). The synthesized catalyst was used in the reduction of Methyl Orange (MO) and Methylene Blue (MB) at room temperature. The Ag NPs/ Mespilus germanica kernel showed excellent catalytic activity in the reduction of these organic dyes. In addition, it was found that Ag NPs/ Mespilus germanica kernel can be recovered and reused several times without significant loss of catalytic activity (**Scheme1**).



Scheme1: Synthesis and evaluation of catalytic activity of Ag NPs/ Mespilus germanica kernel.

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Oxidative esterification of aldehydes using cytosine palladium complex immobilized on SBA-15

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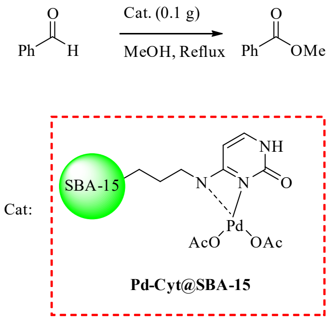
Keywords: Oxidative Esterification, Aldehydes, Cytosine Palladium Complex , SBA-15

Esters are one of the most important fundamental and significant functional group in organic chemistry and chemical industry because they are used in high value products such as cosmetics, surfactant, and food ingredient. In this study, an efficient, economic, and green protocol. A one-pot direct transformation of aliphatic, aromatic, and unsaturated aldehydes into esters in the presence of hydrogen peroxid has been carried out over mesoporoues SBA-15 supported palladium nanocatalyst (Pd-Cyt-SBA-15) under reflux condition.. Pd-Cyt-SBA-15 nanocatalyst demonstrated excellent reusability and stability and could be recycled up to five times whitout loss of significant reactivity The present work benefits of mild reaction conditions, high efficientcy, simple product isolation and shorter reaction times.(scheme1).



Scheme1: Oxidative esterification of aldehydes using cytosine palladium complex immobilized on SBA-15.

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Structural comparison of cubic and hexagonal up-conversions

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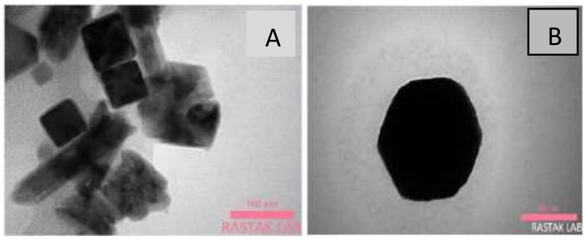
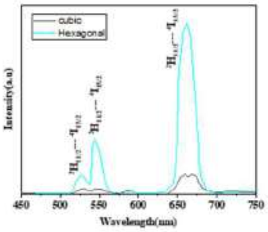
Keywords: Up-conversion, Hexagonal, Hydrothermal

Nanocomposite up-conversion of NaYF4:Yb:Er was synthesized by hydrothermal methods[1]. These nanoparticles were synthesised in different alkaline and acidic environments, at varying temperatures and molar ratios of reactants. Analysis with XRD confirmed the synthesis of hexagonal and cubic structures. TEM analysis was performed to verify the synthetic structures. Then, a comparison was made between cubic and hexagonal synthetic structures as follows: Fluorescence Intensity: Typically, the cubic structure exhibits lower fluorescence intensity compared to the hexagonal counterpart. This is attributed to the higher symmetry of the cubic structure, leading to non-radiative decay pathways that reduce the fluorescence efficiency.

In the hexagonal structure, the crystal field effects can lead to altered energy levels and transitions between the erbium ions, contributing to the up-conversion process and resulting in more intense fluorescence emission. This enhancement is attributed to the lower symmetry of the hexagonal lattice, which promotes radiative decay pathways and increases the efficiency of up-conversion luminescence[2] .The hexagonal structure of NaYF4:Yb:Er supports a photon cascade mechanism, where multiple photon absorption and emission processes occur sequentially, leading to efficient up-conversion luminescence and higher fluorescence intensity.



Scheme1: TEM images of $NaYF_4:Yb^{3+}/Er^{3+}$ UPCN prepared. A:Cubic, B:Hexagonal



Scheme2: Emission spectrum (Photoluminescence spectra) for UPCN nanoparticles under (980nm) excitation

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Optimization of operational parameters to remove arsenic ion from aqueous solutions by functionalized magnetic SBA-15 nanoadsorbent

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Keywords: Santa Barbara amorphous-15, Magnetic nanoadsorbent, Adsorption

Arsenic (As) is a metalloid that not only negatively impacts human health but also irreversibly damages nature and the health of biological species. Therefore, removing this toxic ion from the ecosystems is absolutely vital [1]. In this research, a nanocomposite with a core-shell structure consisting of $MnFe_2O_4$ magnetic nanoparticles as the core and mesoporous silica SBA-15 silicate functionalized with adenine nucleobase (Ade) as the shell was synthesized and used as a mesoporous nanosorbent to remove As(V) from aqueous solutions [2]. Operational parameters for the As(V) adsorption, such as pH, adsorbent amount, contact time, temperature, and initial ion concentration, were investigated using batch experiments. Results showed that the best absorption, which was equal to 96%, occurred at pH 6, temperature of 298 K using 0.8 g L^{-1} of nanoadsorbent in 10 mg L^{-1} of initial As(V) solution during 60 min (Figure 1).

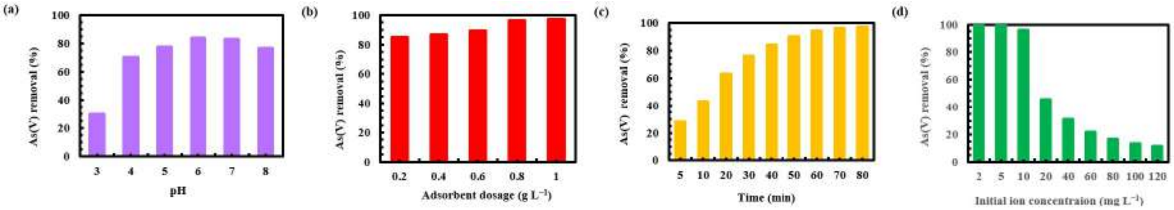

Figure 1: Effect of (a) solution pH, (b) adsorbent dosage, (c) contact time, and (d) initial ion concentration on the removal efficiency of the As(V) ion.

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Kinetic study of arsenic adsorption onto functionalized magnetic SBA-15 nanoadsorbent in aqueous media

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Keywords: Arsenic removal, Adsorption kinetics, Manganese ferrite

It's important to remove arsenic contaminants from wastewater since arsenic in the aquatic environment can pose serious health risks to people. This investigation explored the adsorption kinetics of As(V) ion on the magnetic SBA-15 functionalized with adenine nucleobase [1]. Batch experiments were conducted at various contact times ranging from 5 to 80 minutes. 25-mL solutions containing 10 mg/L of As(V) ions were prepared and adjusted to an optimal pH of 6. Adsorption experiments were carried out at 298 K using 20 mg of adsorbent. The solutions were agitated at 200 rpm in a shaker. After a specified contact time, the adsorbent was separated from the solution, and the residual arsenic concentration was determined using atomic absorption spectroscopy. The results showed a rapid initial adsorption rate due to numerous vacant adsorption sites on the nanoadsorbent. However, as contact time increased, the rate decreased. Equilibrium was reached after approximately 60 minutes, suggesting that further contact time did not enhance the adsorption capacity [2]. The adsorption kinetics of As(V) ions onto nanoadsorbents were studied using pseudo-first-order and pseudo-second-order kinetic models (Figure 1 a,b). The pseudo-second-order model was found to be more accurate, indicating chemisorption.

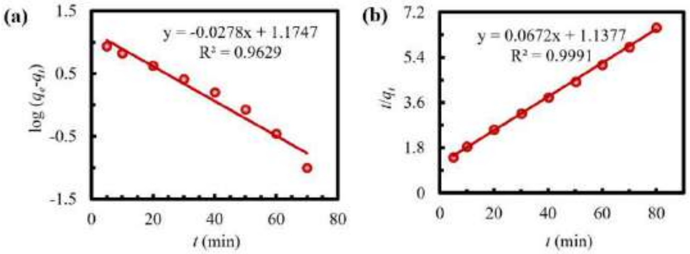

Figure 2: Linear plots of (a) pseudo-first-order and (b) pseudo-second-order kinetics models.

References

[1] Badvi Loulic, F.; Haji Seyed Mohammad Shirazi, R.; Miralinaghi, M.; Ahmad Panahi, H.; Moniri, E. Highly efficient Removal of toxic As(V), Cd (II), and Pb(II) ions from water samples Using $MnFe_2O_4$@SBA-15-$(CH_2)_3$-Adenine as a recyclable bio-nanoadsorbent. *Microporous Mesoporous Mater.,* 2023, 356, 112567.

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The effect of adsorbent surface modification on arsenic removal efficiency using manganese ferrite-based nanoparticles from aqueous media

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Keywords: Toxic ion, Adsorption process, Magnetic nanoadsorbent

To study the effect of surface modification on As(V) removal efficiency, the adsorption performances of three prepared materials in our previous work [1], $MnFe_2O_4$, $MnFe_2O_4$@SBA-15, and $MnFe_2O_4$@SBA-15@ $(CH_2)_3$-Ade, were compared. The results are presented in Figure 1. Under the same conditions, $MnFe_2O_4$@SBA-15@ $(CH_2)_3$-Ade adsorbent had a higher removal efficiency compared with other unmodified adsorbents. It implies that the adenine (Ade) coating served as a main coordination site for metal ions due to the existence of nitrogen atoms and conjugated aromatic rings in its molecular structure. Amine group (—NH_2) in Ade may play a prominent role in arsenic exclusion via participation and complexation interactions [2].

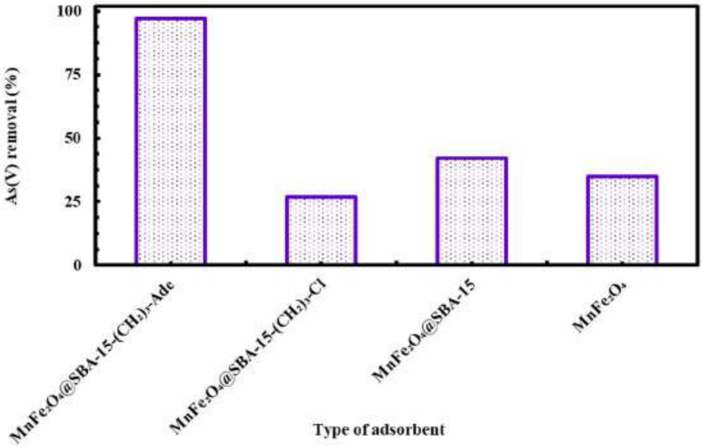

Figure 1: Effect of surface modification on the removal efficiency of As(V) (10 mg L^{-1}).

References

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Synthesis and characterization of Mg-Fe layered double hydroxide

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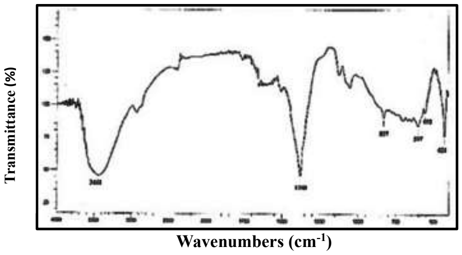
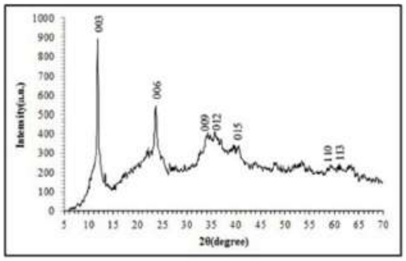
Keywords: LDH, Mg-Fe, XRD, FT-IR

Layered double hydroxides (LDHs) belong to a general class called anionic clay minerals. The general chemical formula of LDH clays is written as:$[M^{II}_{1-x}M^{II}_{x}(OH)_2]^{x+}$ $(A^{n-})_{x/n}.yH_2O$ where M^{II} is a divalent metal ion, such as Mg^{2+},Ca^{2+},Zn^{2},etc, M^{III} is a trivalent metal ion, such as Al^{3+},Cr^{3+},Fe^{3+},Co^{3+},etc and A^{n-} is an anion , such as Cl^{-},CO_3^{2-}, NO_3^{-},etc. Mg-Fe-LDH was obtained by co-precipitation method at hydrothermal condition. The prepared LDH was characterized by X-ray diffraction(XRD) and fourier transform infrared spectrometer(FT-IR). The XRD patterns exhibit the characteristic reflections of LDHs with a series of (003), (006), and (009) diffraction peaks, with 2θ of the (003)peak is 9.70 and according to this value we can calculate the basal distance, 4.58A°. In the FT-IR spectra, an intense and broad adsorption band located at 3444 cm^{-1} was observed, which was attributed to the OH stretching due to the presence of hydroxyl groups and interlayer water molecule of LDH. The absorption peaks at 1380 and 827 cm^{-1} are due to the presence of nitrate ions. In comparision to normal liquid water, the band has shifted towards lower wave numbers by about 20 cm^{-1}, indicating that this water is present in the LDH interlayer. In the low frequency region, the adsorption peaks correspond to the lattice vibration modes(Fe-O, Mg-O, Mg-O-Fe).



Scheme1: FT-IR spectra of Mg-Fe-LDH.



Scheme2: The XRD pattern of Mg-Fe-LDH

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Selective oxidation of alcohols to carbonyl compounds catalyzed by vanadium schiff base complexe under mild conditions

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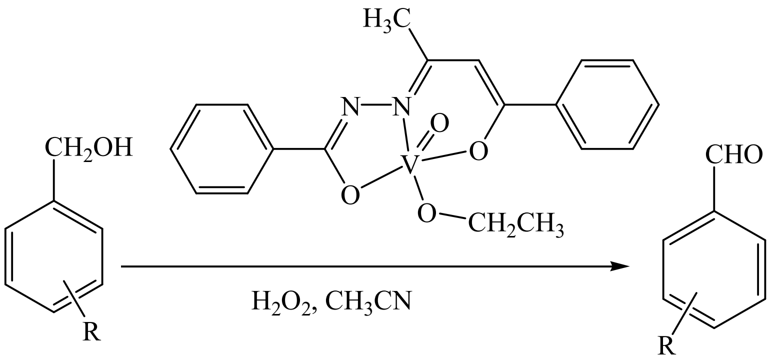
Keywords: Vanadium Schiff base, Alcohole, Aldehyde, Catalyst, Oxidation

The selective oxidation of alcohols to corresponding aldehydes or ketones is fundamental and important in organic synthesis. For example, benzaldehyde and vanillin are widely used in the production of agrochemicals, pharmaceuticals, fragrances and fine chemicals [1].

Recently many investigations have been performed about catalytic behavior of Schiff- base complexes in order to simulation their enzymetic effect and also further finding of biomimetic reactions of cytochrome P-450 enzymes [2].

In this work, first (E)-N'-bis(4-oxo 4-phenyl butane-2-ylidene) benzohydrazide was prepared by the reaction of benzoyl acetone with benzohydrazide. Then, the vanadium Schiff base complexe (V(O)L) was prepared by the reaction of (E)-N'-bis(4-oxo 4-phenyl butane-2-ylidene) benzohydrazide with bis(acetylacetonato)oxovanadium (IV). Also, the ligand and complex were characterized by spectroscopic methods such as IR ،^{1}H NMR ،^{13}C NMR and x-ray crystallography. (V(O)L) was used as a catalyst for the efficient oxidation of alcohols with hydrogen peroxide (**Scheme1**). Various reaction parameters were optimized for the reaction of benzyl alcohol.



Scheme1: General procedure for oxidation of alcohols with hydrogen peroxide.

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Selective Oxidation of Sulfides Catalyzed by a Mn(IV) Schiff-Base Complexe Under Mild Conditions

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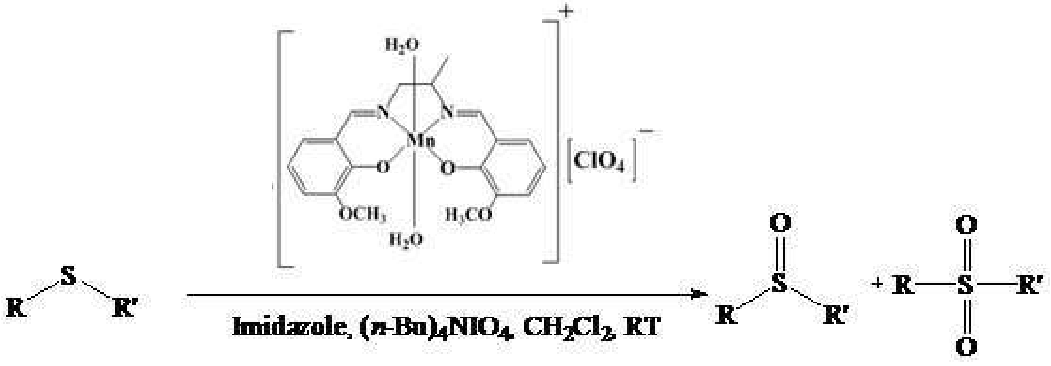
Keywords: Manganese(III) Schiff base, Sulfoxide, Sulfone, Catalyst, Oxidation

Organic sulfoxides and Sulfones are useful synthetic intermediates for the construction of various chemically and biologically active molecules. They often play an important role as therapeutic agents such as anti-ulcer (proton pump inhibitor), antibacterial, antifungal and anti-atherosclerotic [1].

The oxidation of sulfides is the most straightforward method for the synthesis of sulfoxides and Sulfones. Recently many investigations have been performed about catalytic behavior of Schiff- base complexes in order to simulation their enzymetic effect and also further finding of biomimetic reactions of cytochrome P-450 enzymes [2].

In this work, Mn(III) Schiff base complex was prepared by the reaction of *N,N*′bis(2-hydroxy-3-methoxy benzaldehyde)-1,2-propan diimin with $Mn(OAc)_2.4H_2O$. Also, the complex was characterized by spectroscopic methods. The complex was used as a catalyst for the efficient oxidation of sulfides with tetrabutylammonium periodate. (**Scheme1**). This investigation results in: Reducing reaction time of oxidation of sulfides, Increasing catalytic system yield, Increasing selectivity.



Scheme1: General procedure for oxidation of sulfides with tetrabutylammonium periodate.

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Effective sulfide oxidation catalyzed by molybdenum Schiff base complex under mild conditions

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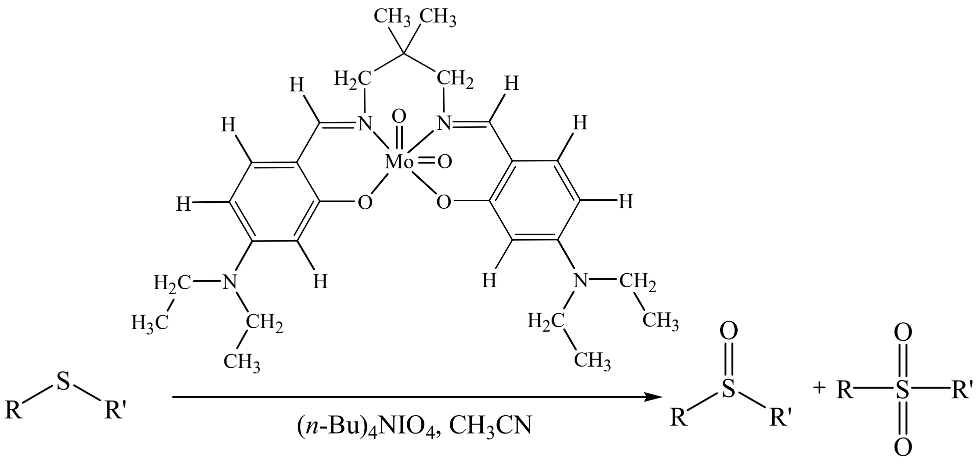
Keywords: Molybdenum Schiff base, Sulfoxide, Sulfone, Catalyst, Oxidation

The selective oxidation of sulfides to sulfoxides and sulfones is a chemical transformation of great importance, both for organic synthesis and for the development of new drugs and materials. [1].

Recently many investigations have been performed about catalytic behavior of Schiff- base complexes in order to simulation their enzymetic effect of cytochrome P-450 enzymes [2]. In this work, first *N, N′*bis(4-diethylamino salicylidine)-2,2-dimethyl-1,3- propanediamine was prepared by the reaction of 4-diethylamino salicylaldehyde with 2,2 dimethyl 2,3 propandiamine. Then, the molybdenum Schiff base complex was prepared by the reaction of *N, N′*bis(4-diethylamino salicylidine)-2,2-dimethyl-1,3- propanediamine with bis(acetylacetonato)dioxomolybdenum(VI). Also, the ligand and complex were characterized by spectroscopic methods such as IR ،^{1}H NMR and x-ray crystallography. The complex was used as a catalyst for the efficient oxidation of sulfides with tetrabutylammonium periodate **(Scheme1)**.



Scheme1: General procedure for oxidation of sulfides with tetrabutylammonium periodate.

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Activated carbon/MoO_3 as a highly efficient catalyst for green synthesis of spiro[3,4']1,3-dihydro-2*H*-indol-2-one-4',6',7',8'-tetrahydro-2',5'(1'*H*,3'*H*)-quinazoline-diones

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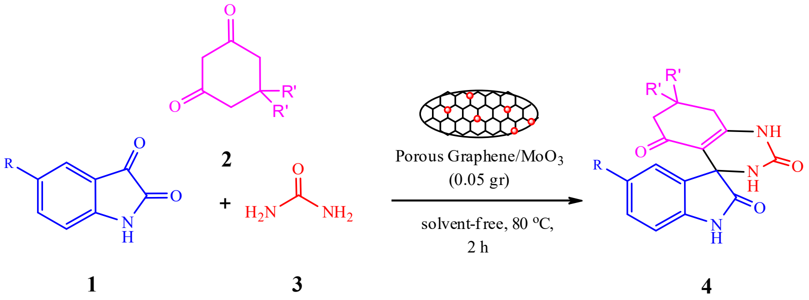
Keywords: Activated carbon/MoO_3 nanocomposite, Catalyst recyclability, Green procedure, Solvent-free

In recent years, much attention has been paid by scientists to expand the different applications of new nanocomposites which have been successfully synthesized based on graphitic materials due to their important impressive classes of carbon nanostructures (for instance, fullerenes, *activated carbon*, carbon nanotubes, nanofibers, and etc.) [1]. In this study, the activated carbon/MoO_3 nanocomposite was prepared through a known procedure [2], characterized and applied as a highly efficient heterogenous catalyst for the synthesis of spiro[3,4']1,3-dihydro-2*H*-indol-2-one-4',6',7',8'-tetrahydro-2',5'(1'*H*,3'*H*)-quinazoline-diones in high yields *via* a Biginelli-type reaction of isatins **1**, 1,3-cyclohexanediones **2** and urea **3**, at 80 ˚C under solvent-free conditions (Scheme 1).



Scheme 1: Synthesis of spiro[3,4']1,3-dihydro-2*H*-indol-2-one-4',6',7',8'-tetrahydro-2',5'(1'*H*,3'*H*)-quinazoline-diones (**4a–h**) using an activated carbon/MoO_3 nanocomposite as catalyst.

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Unexpected preparation of polythiocyanogen (SCN)n in the solid state at room temperature

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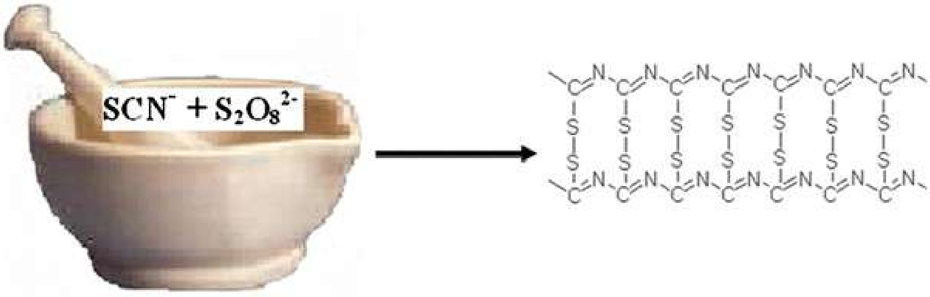
Keywords: Polythiocyanogen, Mechanochemical, Peroxydisulphate, Thiocyanate

The oxidation of thiocyanate in an aqueous solution is often complicated by the varied oxidation state of sulphur and the relative redox instability of cyanide. The oxidation of thiocyanate to polythiocyanogen by peroxydisulphate was carried out in a solid phase reaction at room temperature. In the solid-phase chemical oxidation of thiocyanate by peroxydisulphate the amorphous polythiocyanogen is generated. During the transformation of the reactants into products, the changes were studied by scanning electron microscopy (SEM). The products were characterised by gel permeation chromatography (GPC), IR, UV- visible spectroscopy, X-ray powder diffraction, SEM, and EDX. The results of the chromatogram indicate that the polythiocyanogen is monodisperse and oligomer nature containing broad bimodal peaks with low molecular fractions.



Scheme1: Mechanochemical preparation of polythiocyanogen.

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Synthesis of bimetallic yttrium-copper-metal-organic framework based voltammetric sensor

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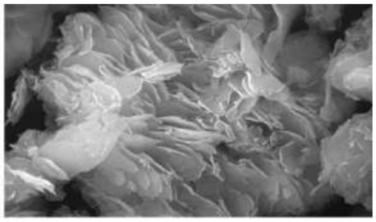
Keywords: Dopamine, Uric acid, Modified electrode, Electrochemical sensor, Y-Cu-MOFs

In this work, bimetallic yttrium-copper metal-organic frameworks (Y-Cu-MOFs) are fabricated via a solvothermal strategy. The Y-Cu-MOFs were characterized using Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), Field emission-scanning electron microscope (FE-SEM), Transmission electron microscope (TEM), Energy-dispersive X-ray spectroscopy (EDS) and elemental mapping analysis (Scheme 1). Then a voltammetric dopamine sensor was created based on a carbon paste electrode modified with bimetallic Y-Cu-MOFs (Y-Cu-MOFs/CPE). Under optimal conditions, the Y-Cu-MOFs/CPE sensor demonstrates superior detection capabilities, with a broad linear range to DA from 0.1 to 400.0 μM and a limit of detection (LOD) of 0.032 μM. Also, the differential pulse voltammetry method (DPV) was utilized for the analysis of DA in the presence of uric acid (UA). DPV results indicated that the peak-to-peak separation of DA and UA was 170 mV at the Y-Cu-MOFs/CPE. Finally, the practical feasibility analysis demonstrates a recovery of 95.7% and 104.3% for DA and UA in dopamine injection and urine specimens [1,2].



Scheme 1. FE-SEM images of Y-Cu-MOF.

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Synthesis of magnetic bentonite-supported metformin-Cu(II) complex as a recyclable catalyst for water treatment

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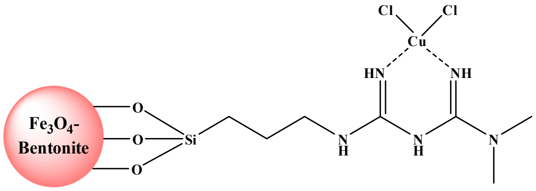
Keywords: Bentonite, copper complex, metformin, water treatment

The application of bentonite, which has received much attention as a natural adsorption material and catalyst support, has many advantages, such as easy separation and reusability [1]. During the last few years, many researchers have focused on magnetic heterogeneous catalysis techniques instead of homogeneous catalysts using natural supports such as bentonite for chemical transformations [1]. Improved wastewater treatment is essential to ensure the health of humans and ecosystems [2]. Wastewater treatment significantly reduces the disease risk by removing harmful substances from effluent [2]. In this study, a novel method is applied to synthesize magnetic bentonite-supported metformin-Cu(II) complex as an efficient and magnetically recyclable catalyst for water treatment (Scheme 1). The prepared catalyst was characterized by FTIR, XRD, SEM, TEM, VSM, TGA/DTG, BET, EDS, and elemental mapping and applied for the reduction of organic dyes and 4-nitrophenol at room temperature in aqueous media.



Scheme 1: The proposed structure of Fe_3O_4-Ben@Met-Cu(II).

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Nanocomposite active packaging films including bacterial cellulose, guar gum, TiO_2 nanoparticles and cardamom essential oil for preserving salmon fish

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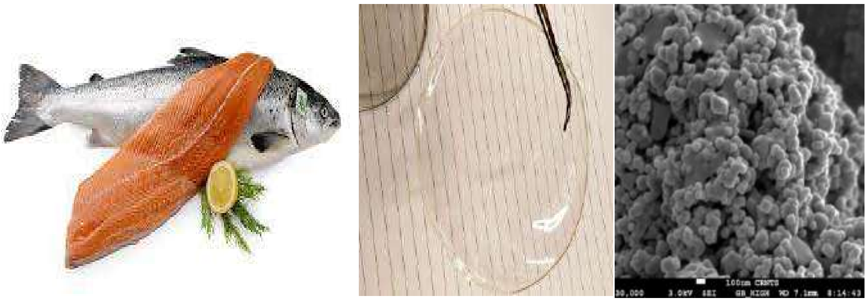
Keywords: TiO_2 nanoparticles, Cardamom essential oil, Salmon fish, Bacterial cellulose

Titanium dioxide nanoparticles (TiO_2 NPs) have numerous biomedical applications because of their distinctive antioxidant, antibacterial, antifungal, anticancer, larvicidal, antibiofilm, antileishmanial, and photocatalytic properties [1]. TiO_2 NPs can provide UV protection to active films or edible coatings, delaying food oxidation caused by UV light [2]. This study developed a composite film for packaging refrigerated common carp fillets using bacterial cellulose/Guar gum (GG) base with the addition of TiO_2 NPs and cardamom essential oil (CEO) (**Scheme 1**). The incorporation of CEO and TiO_2 NPs in composite films increased their antimicrobial and antioxidant properties. In conclusion, this bioactive nanocomposite film significantly increased the shelf life of refrigerated fish fillet samples for 12 days by inhibiting microbial growth and reducing the oxidation rate compared to the control sample. The knowledge obtained from this study shows that film incorporation with TiO_2 NPs increases the shelf life of food products.



Scheme 1. Effect of TiO_2 NPs incorporation with composite films in preserving fish.

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Synthesis and Characterization of an Innovative Magnetic Triazine-Based Covalent Organic Framework for Enhanced Dye Removal Efficiency

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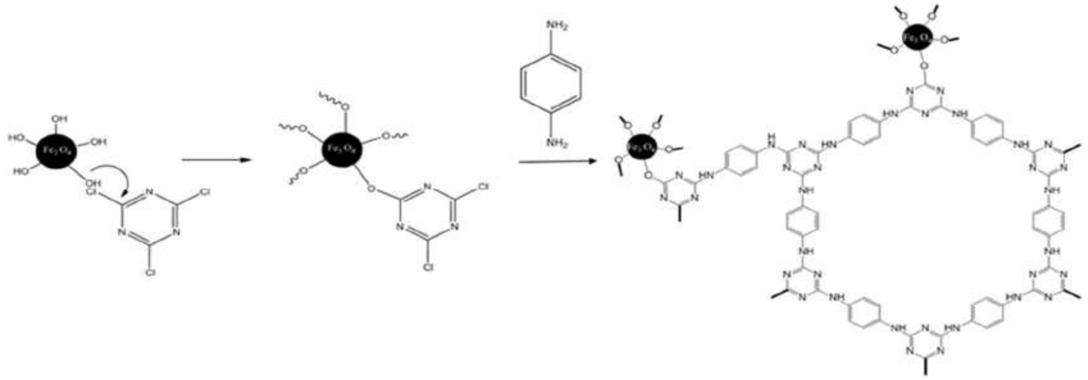
Keywords: Magnetic Triazine-Based Covalent Organic Framework (MTCOF), Dye Removal, Azo Dyes

The issue of dye removal from industrial wastewater is a significant environmental concern and, therefore, has garnered considerable attention from researchers [1]. To address this challenge, various adsorbents have been employed with notable efficiency [2]. This study involved the preparation of an efficient and novel Magnetic Triazine-Based Covalent Organic Framework (MTCOF) nanocomposite for this purpose. Comprehensive characterization of the adsorbent was performed using FT-IR spectroscopy, SEM, EDX, VSM, XRD, BET surface area analysis, and zeta potential measurements. The MTCOF adsorbent was evaluated for its efficacy in removing toxic azo dyes of Janus Green (JG) and Malachite Green (MG) cationic dyes from environment water samples. The study investigated the impact of critical operating parameters such as the pH of the solution, duration of contact, amount of adsorbent used, and volume of the sample on dye removal efficiency.



Scheme1: Synthesis and structure of the nanocomposite.

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Exploring the Properties and Applications of Nano Azide Complexes in Inorganic Chemistry

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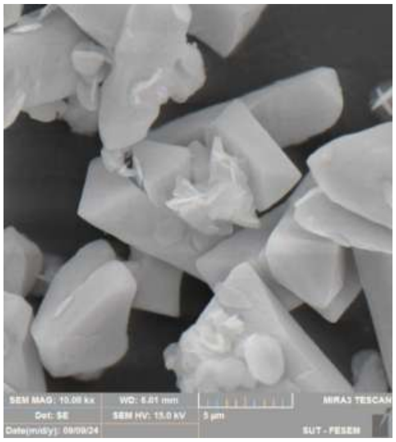
Keywords: Azide, Nanotechnology, Nano complexes

Among the widely used bridging groups, azide has a very rich chemical composition and magneto chemistry, which can bind metal ions in different states and transmit magnetic exchange of different nature and magnitude. In chemistry, compounds containing azide are important due to their versatile applications, especially explosives and propellants in airbags. [1,2]

In this research, using an ultrasonic bath with raw materials Acetohydrazide, Sodium azide, Lead(ll) acetate, a new nanocomplex of azide was produced. The IR test was taken from the sample and it was matched with the spectrum of acetohydrazide ligand. Also, the SEM test results Indicator was nano plates flower-like with thickness less than 26 nm (**Scheme1**).



Scheme1: Image of nano azide complex.

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Synthesis and identification of metal-organic nanocomposites containing nitrogen-donating ligands

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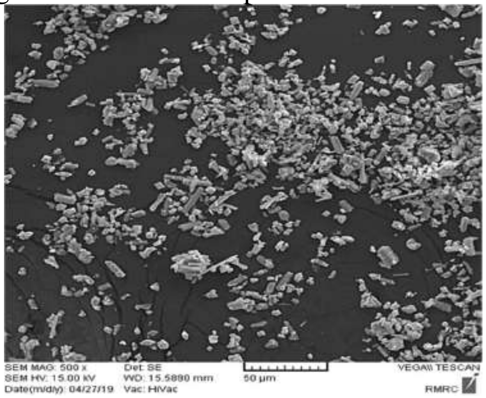
Keywords: Nitrogen donor, Metal-Organic, Nano Structure, Identification

The physicochemical properties of materials are controlled by the synergistic effects of structures and compositions, and MOFs are amazing examples of how the unique structure of hollow-core materials can provide a set of beneficial properties. Among them, the ratio of surface to volume has increased. low density; reactor microenvironment; higher loading capacity; and has reduced the length of mass and load transfer [1,2]. Using the required materials and solvents such as zinc nitrate, pyridine 2-carbaldehyde, pyridine 4-carboxylic acid hydrazide from Aldrich and ethanol solvent from Merck and laboratory devices used in this project such as FT-IR device and the intended ligand was identified by scanning electron microscope (SEM). New metal-organic compounds containing nitrogen donating ligands with hydrazone ligand were synthesized and identified by FT-IR spectrum. The structure of the compound was determined by X-ray crystallography. Nanoparticles of the above composition were synthesized by the reaction method under ultrasonic waves. The morphology and structure of these nanocomposites were studied using a scanning electron microscope (SEM) (**Scheme**). Weak interactions which is important in determining the network arrangement of this compound, was investigated. Also, weak interactions between coordination chains can determine the network arrangement of these compounds.



Scheme: SEM image of the nanostructure of the desired compound.

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Performance of polycarboxylate ether and lignosulfonate organic additives and their effect on cement particles as a mineral and improving compressive strength, durability and reliability of concrete

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b) Bachelor of Chemical Engineering, quality control manager of mortar factory ready
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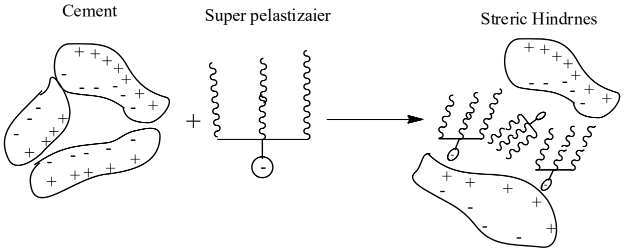
d) Senior expert in organic chemistry, expert in Nizar Cement Chemistry Laboratory, Qom

Keywords: Durability, Cement particles, Electrical resistance, Water absorption, Chloride ion

Production of concrete with long life and high resistance in the construction of projects such as oil wells, dam construction, paving roads and airports, bridges and other concrete structures without using super-lubricants based on carboxylate, lignosulfonate, etc. as material Organic is not possible, which indicates the use of this substance. With the synthesis of this material, it is possible to make a very important contribution to the environment, because the strength of concrete can be obtained by using large polycarboxylate molecules, with the water reduction mechanism, and the increase of cement in concrete can be prevented, for every one ton of cement About one ton of carbon monoxide enters the air. It is also possible to increase durability and life span, which is a step towards sustainable development. In this research, using lignosulfonate and polycarboxylate additives, the durability and useful life of concrete in terms of permeability, capillary water absorption, chloride ion penetration, and electrical resistance have been investigated with the Wenner device, and the effect of an organic substance on the material, a cement mineral has been studied. Figure 1 shows this effect.



Scheme1: Super plasticizer performance on cement particles.

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The Effect of calcination temperature on the structure of $Bi_2Fe_4O_9$ nanoparticles prepared by thermal treatment

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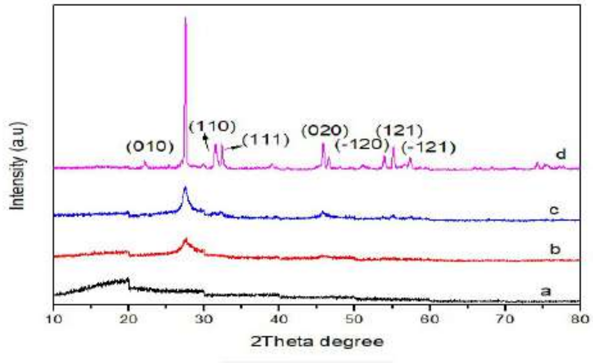
Keywords: Bismuth ferrite, Calcination, Thermal treatment

The present work, the synthesis of $Bi_2Fe_4O_9$ nanoparticles prepared by thermal treatment and the effects of calcination temperature on their formations are reported for the first time .Metal nitrate reagents were used as precursors , polyvinyl pyrrolidone (PVP) was used as the capping agent, and deionized water was used as the solvent. An aqueous solution of PVP was prepared by dissolving 3.5 g of polymer in 100 ml of deionized water at 80°C, then mixing iron nitrate and bismuth nitrate into the polymer solution and constantly stirring for 2h using a magnetic stirrer until an orange solution was obtained. The mixed solution was poured in to aglass Petri dish and heated at 100 $^{\circ}$ C in an oven for 24 h to evaporatethe water. The calcination of the powder was conducted at 723º,773 ^{0},823 ^{0}k for 3 h for the decomposition of organic compounds and the crystallization of the nanocrystals. The nano structure of the $Bi_2Fe_4O_9$ nanoparticles was characterized by the XRD technique. [1-3]



Scheme1: XRD patterns of $Bi_2Fe_4O_9$ precursor and nanocompositecalcined at (a)273, (b) 723, (c)773, and (d) 823^{0} K.

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Preparation of New Nano Inorganic materials and Study of Their Biological Properties: (Anti-Cancer and Antibacterial) & There's Plenty of Room at the Bottom

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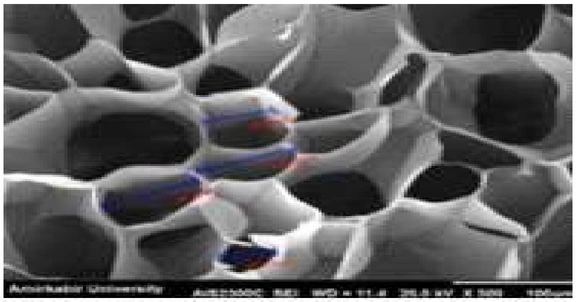
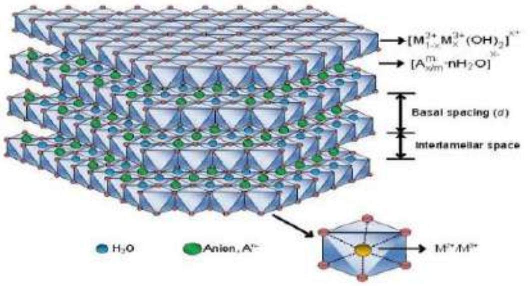
Keywords: Nano, Carriers, Inorganic, Biological, Anticancer

Nanomaterials have the potential to use as drugs design and delivery systems. In this abstract, a number of the new nano materials were prepared. These materials have different and various composition from mononuclear to multinuclear complexes and Layer double hydroxide compounds. These new materials were characterized by spectroscopic methods such as FT-IR and UV spectra, X-ray diffraction, SEM techniques and some physical properties. The biological activities such as antitumor activities of these nano compounds against a different kinds of tumor cells such as panel of human tumor cell lines (HT29: Human colon adenocarcinoma cell line T47D: human breast adenocarcinoma cell line) was determined by MTT(3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyl-tetrazolium bromide) assay. The antibacterial of these compounds were studied on a number of bacterial colonies such as Escherichia coli, *Klebsiella pneumonia* and two Gram-positive species. [1,2] **HOW CAN WE USE FROM THESE POINTS FOR APPLICATION IN OUR COUNTRY SPECIALLY IN INDUSTRY?**





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Synthesis of yttrium-zinc metal−organic framework for voltammetric sensing epinephrine

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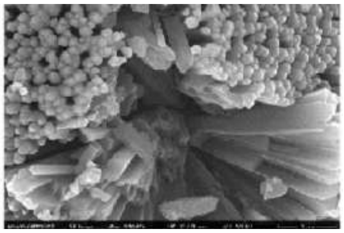
c) Environment Department, Institute of Science and HigTechnology and Environmental Sciences, Graduate University of Advanced Technology, Kerman, Iran.

Keywords: Modified electrode, Metal-organic frameworks, Epinephrine, Acetaminophen, Voltammetry

In this work, a voltammetric sensor has been designed for detecting epinephrine (EP). This sensor utilizes a bimetallic yttrium-zinc metal-organic framework (Y-Zn-MOFs) to modify a carbon paste electrode (Y-Zn-MOFs/CPE), aiming to enhance conductivity and improve the charge transfer rate. The electro-catalytic performance of the Y-Zn-MOFs/CPE sensor was analyzed using cyclic voltammetry (CV), revealing improved performance compared to the un-modified electrode. The Y-Zn-MOFs significantly enhance the electro-catalytic activity towards EP. The Y-Zn-MOFs/CPE sensor exhibited a wide linear dynamic range from 0.01 to 700.0 µM, with low limit of detection (LOD) of 0.003 for EP. Moreover, Differential pulse voltammetry (DPV) results indicated that the peak-to-peak separation for EP and acetaminophen (AC) was 170 mV at the Y-Zn-MOFs/CPE. This suggests that the proposed electrode can simultaneously and selectively detect both compounds. It can also be utilized for detecting EP and AC in real specimens, achieving a recovery of 96.7-103.3%. This demonstrates a promising application potential for the electrochemical EP and AC detection [1,2].

Scheme 1. TEM images of Y-Zn-MOF



Scheme 2. FE-SEM images of Y-Zn-MOF

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Application of active packaging base on poly(3-hydroxyalkanoate)/Linseed oil /MgO nanoparticles for increased shelf-life of cherry tomatoes

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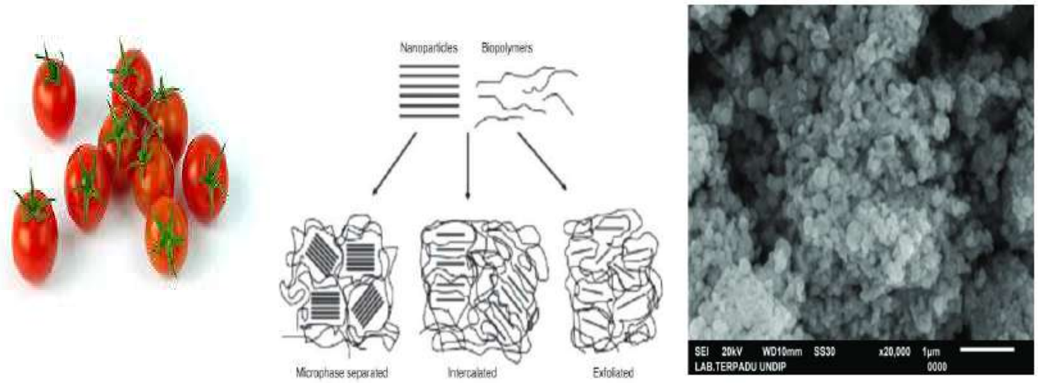
Keywords: MgO nanoparticles, Linseed oil, Cherry tomato, Active packaging

MgO nanoparticles (MgO NPs) are an inorganic compound that has high antibacterial properties against Gram-positive and Gram-negative bacteria (Bacillus and Pseudomonas) [1] MgO is a promising agent for degradable food packaging films. MgO can be synthesized through the green synthesis pathway [2]. This work assessed the effectiveness of an active and eco-friendly poly(3-hydroxyalkanoate) (PHA) based film loaded with 5 wt% Linseed oil (LS) and 0.7 wt% MgO NPs prepared via sonication-assisted for storage cherry tomatoes **(Scheme 1)**. The shelf-life cherry tomatoes in this packaging was carried out for 23 days in ambient room conditions, The results showed that the cherry tomatoes stored in PHA/5LS/0.7MgO packaging experienced better preservation of quality than those in other storage groups, with no signs of surface wrinkling, shrinkage, microbial growth, Furthermore, it was found that the migration of MgO NPs from the nanocomposite packaging to cherry tomatoes was negligible.



Scheme 1. Effect of MgO NP incorporation with composite films in preserving tomato.

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University of Qom, Iran

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Nov. 6&7, 2024

Synthesis, Characterization and Catalytic activity of ruthenium(III) complex

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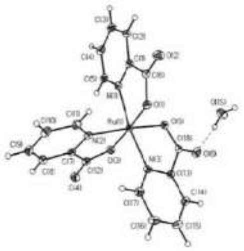
Keywords: Ruthenium(III), CO_2 elimination, crystal structure

Chemists learned a lot in manipulating the intermolecular forces, particularly highly directional metal ligand and hydrogen bonds [1,2]. The ruthenium complexes are amongst the most attractive inorganic compounds due to their varied chemical features, such as redox properties, intense electronic absorption spectra, and generally their rich structural properties [3]. The novel title compound, $[Ru(pyc)_3].H_2O$, where (pycH) is pyridine-2-carboxylic acid was obtained using $(pnH_2)(pydc)$, pn: propane-1,3-diamine pydc: pyridine-2,6- dicarboxylic acid, as proton transfer compound under hydrothermal conditions. Structure of compound (1) shows a very interesting phenomenon i.e. a catalytic CO_2 elimination from starting diacid on ruthenium(III) center, because we started with pyridine-2,6-dicarboxylate as anionic fragment, but pyridine-2-carboxylate was obtained in the crystal structure. Also, the structure shows that the anionic fragment of the starting proton transfer compound is incorporated in the complex and the cation (propane-1,3-diaminium) has been lost. Cell parameters are as follows: a = 30.4062(12), b = 8.4656(3), c = 13.8758(5), β=94.8560(10), V= 3558.9(2), Z= 8, R= 0.021, No. of reflections= 5184. As seen in Scheme1, the ruthenium(III) atom is six-coordinate by three nitrogens including N(1), N(2) and N(3) from pyridine rings and three oxygens including O(1), O(3) and O(5) belonging to carboxylate groups.



Scheme1: The structure of title compound

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Synthesis, characterization and X-ray structure of a Ni(II) complex containing chelidamic acid

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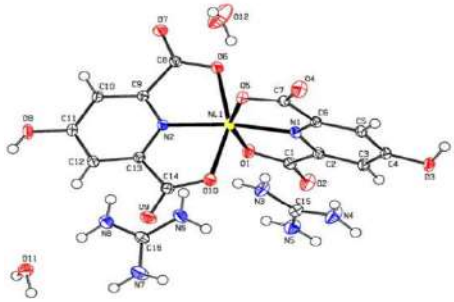
Keywords: X-ray diffractometry; Crystal structure; Chelidamic acid;

Our research group has been concerned with the synthesis of self-associated systems that can function as suitable ligands in the synthesis of metal-organo compounds [1-3]. The novel metallic compound formulated as $(GH)_2[Ni(hypydc)_2]$**.**$2H_2O$, was synthesized from 4-hydroxypyridine-2,6-dicarboxylic acid (chelidamic acid), $(hypydc)^{2-}$ and guanidine (G). This compound crystallizes in triclinic system, $P\bar{1}$; space group. The unit cell dimensions are: a = 8.9253 (6) Å, b = 9.9060 (6) Å, c = 13.2186 (9) Å, α = 101.415 (3)°, β = 103.099 (3)° and γ = 91.938 (3)°. The final R value for this compound is 0.026 for 9650 reflections. The six donor atoms of the two 4-hydroxypyridine-2,6-dicarboxylate or $(hypydc)^{2-}$ ligands form a distorted octahedral arrangement around the Ni^{II} center. In the crystal structure of the title compound, a wide range of non-covalent interactions consisting of hydrogen bonding (of the types of O—H···O and N—H···O with D···A ranging from 2.5901(8) Å to 3.3823(12) Å), ion pairing and C—O···π, N—H···π and C—H···π stacking interactions connect the various components into a supramolecular structure.



Scheme1: The structure of title compound

References

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Optimizing Fule, temperature, pH effect and investigation the Electrochemical behavior of CuNiO nanoparticles

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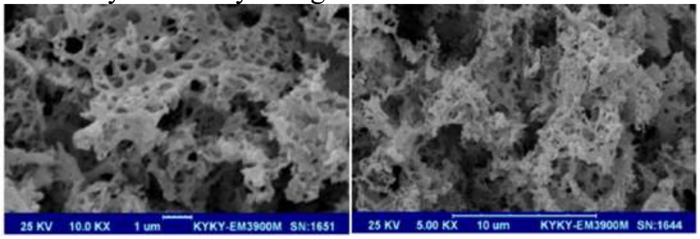
Keywords: Combustion synthesis, Glycine, hexamine, Electron microscope, X-ray diffraction

In this research, the solution combustion synthesis(SCS) of porous oxid nanoparticles $Ni_{0.8}Cu_{0.2}O$ was investigated and optimized. In this method, we first determined the optimal fuel according to the reaction with one fuel (glycine, thiourea, urea, citric acid, hexamine), then according to the synthesis process and the completeness of the reaction, we selected the base fuel and examined it. We paid two fuels at the same time (glycine-citric acid, glycine-urea, glycine-thiourea, glycine-hexamine). According to the synthesis process and identifications, glycine-citric acid fuel (ratio 3:1) was chosen as the optimal fuel. After that, temperature and pH were optimized. All syntheses were identified by infrared spectroscopy (FT-IR) and electron absorption (UV-Vis), and nanoparticles were identified and selected by X-ray diffraction (XRD). According to SEM electron microscope images, the type of morphology of nanoparticles was identified. According to the electron microscope images, nanoparticles have shown a uniform and porous structure according to the optimization done. It should be kept in mind that the goal of this project is to obtain bimetallic porous nanoparticles for better electrochemical activities. This type of porous nanoparticles caused a good catalytic activity on the surface of the carbon paste electrode. Finally, the best nanoparticle was selected according to the optimized conditions and was investigated as a catalyst in electrochemical processes. It was observed that in these porous nanoparticles, the presence of two metals together causes better catalytic activity at higher currents..



Scheme 1. FE-SEM images of $Ni_{0.8}Cu_{0.2}O$.

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Weak interaction Organization in a Novel Cadmium (II) Coordination Compound

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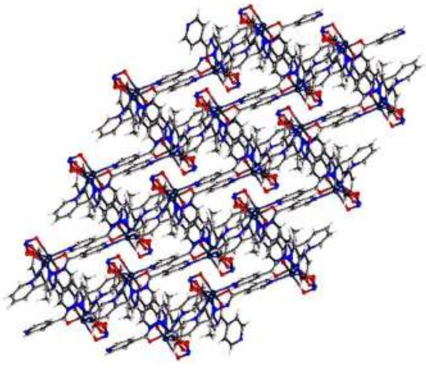
Keywords: Supramolecular, Metal-Organic, 3D Structure, Weak interaction

Supramolecular metal-Organic coordination compounds formed by self-assembly are a frontier in research because of their attractive applications in novel subjects. Weak interactions such as van der Waals forces, dipole‐dipole attractions, hydrogen bonding, π-stacking, and, … can assemble molecular components selectively into metal-organic structural motifs [1]. One of the obvious challenges is the rational and controllable preparation of metal-ligand frameworks, the formation of which is greatly affected by the nature of the metal ions, organic and inorganic ligands, the, counterions, and other factors [2,3]. We report here on the synthesis and crystal structures of cadmium (II) metal-organic coordination compound with flexible hydrazine derivative ligand. The structure was characterized by elemental analysis, FT-IR and X-ray crystallography. The single-crystal X-ray data shows the coordination number in Cd^{II} ions is six, CdN_3O_3. The Supramolecular architecture designed by wonderful strong H-bonds that influenced on fragments translocations and the π–π stacking interactions creating a 3D framework (Fig. 1).



Scheme: 3D supramolecular feature of complex

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Direct Synthesis of Liquefied Petroleum Gas (LPG) from CO_2 using Copper Nanoparticle-Modified SBA-15 Zeolite

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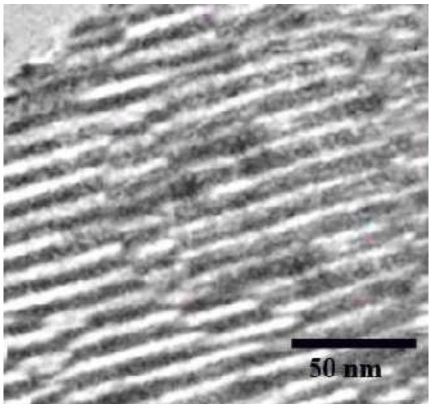
Keywords: Carbon dioxide, Selectivity, Conversion, LPG, Stability

Converting carbon dioxide into hydrocarbons is an innovative solution to reduce greenhouse gas emissions and move towards sustainable fuels. By utilizing the hydrogenation process and selecting the appropriate catalyst, it becomes possible to directly synthesize light hydrocarbons from carbon dioxide [1]. In this research, the direct synthesis of LPG from CO_2 using a hybrid SBA-15 catalyst modified with copper nanoparticles has been investigated. The results show that the modified SBA-15 hybrid catalyst has high catalytic activity and suitable selectivity for LPG production. Results indicated that modifying the catalyst with active copper sites led to a decrease in the catalyst's active surface area [2]. Additionally, TEM results showed that adding CuO oxides resulted in a uniform distribution within the internal channels of the 1Cu/SBA-15 catalyst (Scheme 1).



Scheme1: HRTEM results for 1Cu1Zn/SBA-15.

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Direct conversion of carbon dioxide to light olefins using CeO_2/SAPO-34 zeolite

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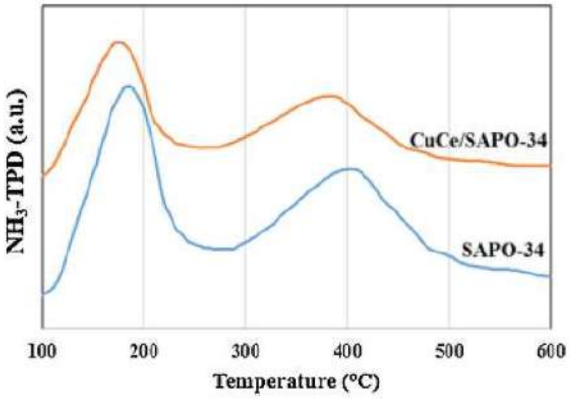
Keywords: Hydrogenation; Selectivity; Light Olefin; Stability

Light olefins such as ethylene and propylene are very important raw materials in the petrochemical industry and are used to produce a wide range of products including plastics, synthetic fibers, rubber, and solvents [1]. The production of light olefins from carbon dioxide is an innovative and sustainable solution to combat climate change and meet the growing needs of the petrochemical industry. In this research, the direct conversion of CO_2 to light olefins over a hybrid catalyst was investigated. The samples were characterized by XRD and NH_3-TPD techniques (Scheme 1). The results showed that the acidity of the modified zeolite decreased [2]. The effect of various factors such as temperature and space velocity on the catalyst performance was studied. Results indicate that the modified hybrid catalyst exhibits high catalytic activity and suitable selectivity for the production of light olefins. The optimal conditions for the production of light olefins were obtained at a temperature of 400 °C and a space velocity of 6 L/g.h.



Scheme1: NH_3-TPD results for synthesized catalyst.

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Investigation of underground water chemistry of the west Qom province and factors affecting

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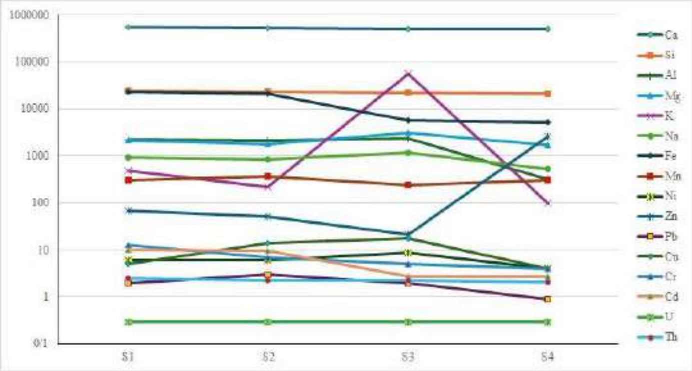
Keywords: Chemistry, Major and Minor Elements, Underground Water, Mineral Deposits, Microorganism

In this study, the chemistry of underground waters of the west of Qom Province have been examined. For this purpose, the elemental characteristics of the samples were analysed using the ICP method. The results of the analysis and field evidence suggest the source of the spring is likely deep underground water. They do not get significant influence from the nearby river. In addition to the basic hereditary characteristics of water (original/primary composition), the outcropped rocks in the area, the activity of faults, the presence of salt lenses and layers rich in some elements underground and the presence of active microorganism masses in the near surface layers appear to be main factors affecting the chemical composition of underground water in the study area.



Scheme1: Linear diagram of element changes in the studied stations.

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Development of a novel three dimensional Zn(II) Metal organic framework: An efficient adsorbent for sustainable Cr(VI) removal

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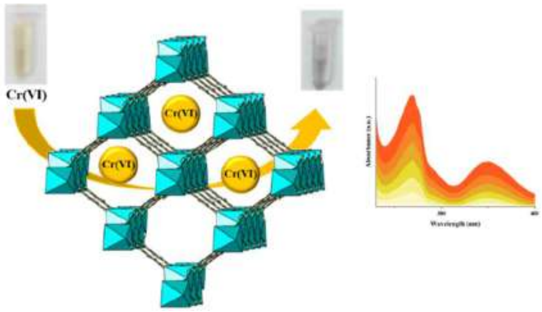
Keywords: Metal-Organic Framework, Adsorption, Cr(VI) removal, Water treatment

Nowadays, environmental issues such as treating the disposed industrial wastewater is an ongoing challenge. Hexavalent chromium, Cr(VI), proved to be among tactical contaminants generally loaded in waste water [1]. Cr(VI) is, particularly hazardous for the human being, causing high risk damages to human body even at trace concentrations [2]. Hence, numerous novel approaches have been established for Cr(VI) elimination. Introduction of metal-organic frameworks (MOFs) as adsorbents open new insights for researchers to overcome existing limitations of Cr(VI) removal [3]. MOFs exhibit specific characteristics such as high surface area, designable pores and modifiable functional groups which make them good candidates as adsorbent [4]. Herein, we investigate a simple route to achieve a 3D Zn based MOFs (CFU-2) through a one-pot solvothermal method (scheme 1). The Cr(VI) removal efficiency of CFU-2 was thoroughly explored. The influence of the primary concentration of the substrate, MOF amount and pH in the removal procedure together with the adsorption mechanism and uptake kinetic of the framework toward Cr(VI) was also studied.



Scheme 1: Structure of CFU-2.

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Synthesis and structural characterization of nano rods lead(II) coordination compound

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Keywords: Lead(II), Nano rods, SEM, Coordination compound

Recently, the development of coordination systems has become increasingly attractive for researchers. Ascetic architecture, luminescence, topologic diversity, magnetic, storage molecular, adsorption, covering, various preparation manners, and other interesting possible usage are among the factors attracting attention and causes for various examinations leading to many researches works in the area of coordination polymers and novel group of material chemistry [1]. Schiff bases that are a significant series of organic ligands have capability of coordination by metal ions for forming stable chelates through N atom of the azo-group as well as other donors. Schiff bases have advantages of simple synthetic pathways, satisfactory biological activity, photochemical features, and high coordination potency, and they include pharmaceuticals and also photoelectric and dye materials [2].

Our present study describes the synthesis and characterization of new nano rods lead(II) coordination compound with hydrazone derivative Schiff base compound. The structure studied by FT-IR, 1Hnmr, 13Cnmr and SEM. The SEM images showed the nano rods morphology for this compound (Figure 1)

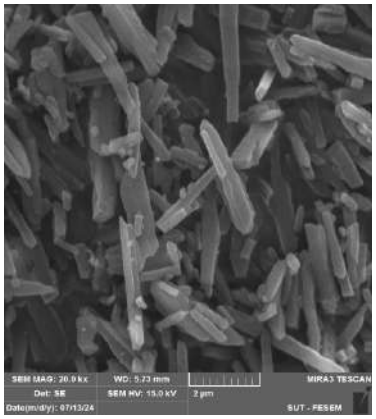

Figure 1. SEM image of the nano rods lead(II) coordination compound

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