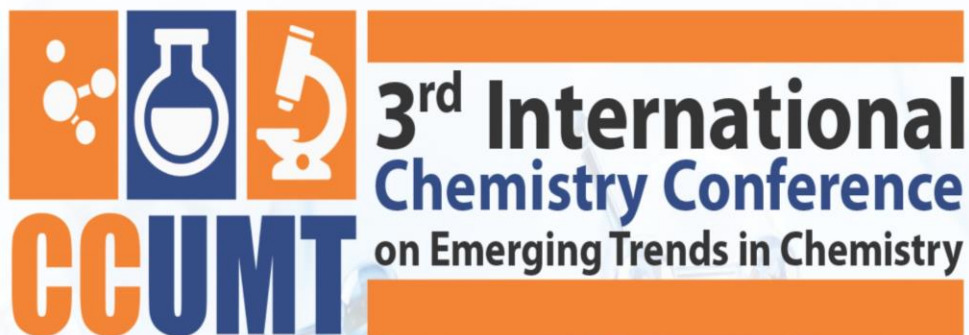


# UMT | SSC

School of Science



April 10-12, 2025

## Abstract Book



Jointly Organized by: Department of Chemistry & Department of Life Sciences, School of Science,  
University of Management and Technology, Lahore, Pakistan.

## PREFACE

*Department of Chemistry, School of Science, University of Management and Technology (UMT) Lahore Pakistan organized the conference on 3rd International Chemistry Conference on Emerging Trends in Chemistry (3rd CCUMT-2025) held from April 10 –12, 2025 at School of Science, UMT, Lahore.*

*This conference was organized to encourage researchers, scientists, engineers, and industry professionals to exchange insights on advancements in Applied and Theoretical Chemistry. Featuring symposia on topics such as Functional Materials, Energy Technologies, Artificial Intelligence, and Environmental Chemistry, 3<sup>rd</sup> CCUMT-2025 seeks to foster interdisciplinary collaboration, explore innovative methodologies, and address contemporary academic and industrial challenges. Themes were Computational Chemistry AI in Chemistry, Analytical, Environmental, Green Chemistry, Organic, Medicinal, Natural Product Chemistry, Inorganic, Material, Nano, Nuclear Chemistry, Applied, Industrial, Polymer, Textile Chemistry, Bio, Nutritional Food, Agricultural Chemistry, Physical, Radio, Electrochemistry.*

*The international speakers from United State of America, United Kingdom, Spain, South Africa, Bahrain and Turkey were attended the conference in hybrid mode online as well as on campus. A total of 250 participants attended the conference, a total of 128 researches were presented related to the conference themes out of which 65 were oral presentations and 63 were poster presentations from all over the Pakistan.*

*Best part was that students from different universities were able to visit under one roof and could interact with renowned national and international scientists. Honorable Governor Punjab (Sardar Saleem Haider Khan) and Dr. Zaib-un-Nisa Hussain (Vice Chancellor, The University of (Home Economics) inaugurated the conference.*

*The Rector UMT, Dr. Asif Raza (S.I (M), H.I. (M)) addressed on significance of event at Inaugural ceremony of conference, and respected DG UMT Mr. Ahmad Abdullah awarded souvenirs and certificates at concluding ceremony.*

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# ORAL PRESENTATIONS

## Elimination of Trace Metals and Drug Residues in Industrial Wastewater by Physicochemical Adsorption on Kaolinite Surface

Simplice Koudjina<sup>1,3\*</sup>, François Zagabe Zabene<sup>2</sup>, Alidor Mbaya Shikika<sup>2</sup>, Fabrice Amisi Muvundja<sup>2</sup>, Guy Y.S. Atohoun<sup>3</sup>, Waris Kewouyemi Chouti<sup>3</sup>

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Heavy metal and drug residues in the environmental have become serious pollutants to be addressed. Grey waters from municipalities, hospitals and chemical industries may be loaded with these chemicals and end up into the environment, especially in water springs, rivers and lakes. Moreover, the pre-treatment measures for these wastewaters are needed to ensure the treated water is environmentally safe and unpolluted. Therefore, we aimed in this work to optimize the physicochemical conditions that favour their adsorption onto Beninese Kaolinite geopolymer from Ketou. Moreover, a quantum chemical mechanistic modeling (VASP code and DFT approach) showed that the adsorption of copper and paracetamol is exothermic according to a single mode for copper with an energy of -139.15 kJ.mol<sup>-1</sup> while that of paracetamol is in two modes, namely the horizontal mode having a high energy of -159.40 kJ.mol<sup>-1</sup>, and the vertical mode of -91.10 kJ.mol<sup>-1</sup>. By heating the kaolinite that had adsorbed these pollutants, it can release them at 435 K and 750 K respectively. This adsorption process does not cause any disorder in its structure ( $\Delta S < 0$ ), as follow the Pseudo-second order model with  $R^2 > 0.99$  and its isotherms are well simulated by Langmuir model. Application to hospital wastewater gave reduction rates in copper of  $90.5 \pm 2.1\%$  and in paracetamol of  $88.5 \pm 3.65\%$ . Kaolinite was

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found to be an effective adsorbent for treating industrial wastewater before its discharge into the environment.



## **Intracellular Penetration of Antibacterial and Anti-Inflammatory Nanoparticles Loaded onto Self-Healing Hydrogels for Enhanced Periodontitis Treatment**

Talia Ghaffar <sup>1,2</sup>, Aqsa Afzaal <sup>1,2</sup>, Mazhar Amjad Gilani <sup>2</sup>, Sobia Tabassum <sup>1\*</sup>

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Periodontitis is a long-lasting inflammatory disease that affects the tissues supporting teeth, making it challenging to eliminate bacteria, reduce inflammation, and promote efficient tissue regeneration. Self-healing hydrogels show promise as alternatives to brittle hydrogels for efficient regeneration. This study aimed to combine antibacterial and anti-inflammatory properties in self-healing hydrogels. The hydrogels were synthesized using gelatin, polyvinyl alcohol, hydroxyapatite, and crosslinkers. Antibacterial polymeric carbon dots (PCDs). They were prepared and functionalized with antibiotics, demonstrating intracellular penetration. Functionalized PCDs and anti-inflammatory polyphenols were incorporated into the hydrogels, which exhibited good in vitro antibacterial and anti-inflammatory activity. Rheological analysis revealed improved mechanical properties, including increased critical strain ratio, self-healing, and reduced viscosity. The hydrogels showed sustained drug release, indicating prolonged therapeutic effects, and degradation and swelling studies showed their good biodegradability and swelling potential. These self-healing hydrogels show great potential as a promising platform for effective periodontitis management, offering combined antibacterial, anti-inflammatory, and intracellular drug delivery capabilities.

## Design, Synthesis and Structural Studies of some New Azoles as Potential Biological Scaffolds

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Azole frameworks serve as privileged scaffolds in the contemporary drug design paradigm owing to their unique physicochemical profile that promotes the development of highly selective, physiological benevolent chemotherapeutics. Several azole nuclei function as bioisostere in medicinal chemistry and prompt the development of tailored therapeutics for targeting the desired biological entities. Besides, the azole scaffold forms an integral part of advanced drug designing methodologies, such as target template in situ drug synthesis, which assists in the rapid identification of the hit molecules from a diverse pool of leads; and direct biomolecule-drug conjugation, along with bioorthogonal strategies that ensure localization, and superior target specificity of the directed therapeutic. Lastly, the structural diversity of the azole framework and high-yielding click synthetic methods provide a comprehensive Structure-Activity Relationship (SAR) analysis for design optimization of the potential drug molecules by fine-tuning the placement of different substituents critical for the activity. Azoles are nitrogen, sulfur, and oxygen-containing compounds with a five-membered ring system that comprises thiadiazole, oxadiazole, triazole, imidazole, isoxazole, pyrazole, and other rings. Mainly known as antifungal agents, azole derivatives demonstrate many other biological properties including anti-diabetic, anti-inflammatory, and anticancer activities. Azoles also show  $\alpha$ -glucosidase inhibition, which includes derivatives of thiadiazoles, oxadiazoles, triazoles, diamine-bridged coumarinyl oxadiazole conjugates with phenylenediamine, benzidine and 4,4'-oxydianiline linkers, and 5,6-diaryl-1,2,4-triazine thiazoles. A new series of 1,3,4-oxadiazoles, 1,2,3-triazoles, pyrazoles and thiazoles have been synthesized and characterized by different spectroanalytical techniques. Fully characterized molecular structures were further studied by single-crystal X-ray diffraction where applicable. Density functional theory calculations at the B3LYP/6-31+G(d) level were performed to compare X-ray geometric parameters, molecular electrostatic potential (MEP), and

frontier molecular orbital analyses of synthesized compounds. MEP analysis revealed that these compounds are nucleophilic.

Moreover, the non-covalent interactions have been characterized using the NCIPLOT index. Frontier molecular orbitals (FMOs) analysis was performed for the evaluation of kinetic stability. All synthesized compounds were screened in vitro for different biological assays and diverse biological trends have been observed in different classes.

## An Overview on Versatile Applications of Glauconite in Chemistry and Biology: A Green Mineral

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Glauconite, a naturally occurring iron potassium phyllosilicate mineral, has garnered significant interest in both chemistry and biology due to its unique structural and compositional properties. Originating primarily in marine sedimentary rocks, this green mineral exhibits a remarkable capacity for ion exchange, adsorption, and catalysis, making it a versatile component in various scientific domains. In chemistry, glauconite's high cation exchange capacity and surface area facilitate its use as an effective catalyst in environmental remediation processes, such as the removal of heavy metals and organic pollutants from wastewater. Its role as a natural ion-exchanger has been leveraged in the synthesis of advanced materials, including nano-composites and zeolites, which are pivotal in catalysis, adsorption, and molecular sieving applications. Also, glauconite's thermal stability and magnetic properties have opened avenues for its use in heterogeneous catalysis and as a component in magnetic materials. In the realm of biology, glauconite's biocompatibility and non-toxic nature have enabled its application in medical and agricultural fields. By understanding and harnessing the multifaceted properties of glauconite, researchers can develop innovative solutions to contemporary scientific and environmental challenges. Furthermore, glauconite's ability to interact with biological molecules has potential implications in drug delivery systems and tissue engineering, where it can act as a scaffold for cell growth and differentiation. This work present to comprehensively explore the diverse applications of glauconite, highlighting its significance in advancing both chemical and biological sciences.

**Keywords:** Glauconite, Catalysis, Ion exchange, Environmental remediation, Nano-composites, Biocompatibility.

## The Role of Theory and Computation in Modern Inorganic Chemistry

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Rapid expansion in hardware capability, combined with new algorithms and, very recently, the emergence of artificial intelligence and machine learning, mean that computation is playing an increasing prominent role in the development of inorganic chemistry. Indeed, the vast majority of papers published in the field now contain some element of theoretical analysis. In this talk I will discuss how theory has enhanced our understanding of experimental data across a range of recent projects from my group. The talk will include cases where we have used the simplest forms of molecular orbital theory that have been in use for over 60 years through to very recent applications of multi-configurational quantum mechanics and machine learning to spectroscopy. I will try to emphasise the value that each of these techniques brings and how they enhance the information content of the experiments.

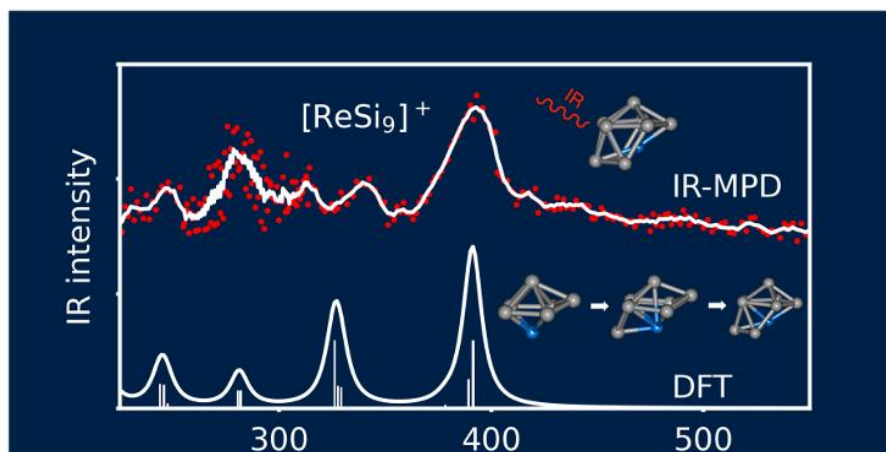


Figure: Comparison of the measured infra-red-multi-photon dissociation (IR-MPD) spectrum of  $[\text{ReSi}_9]^+$  with its DFT-computed counterpart

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**Lasers, Chemistry and the Environment: Scientific Innovation for a Sustainable Planet**

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The integration of lasers in chemistry and environmental science has revolutionized the field, offering innovative solutions for a sustainable planet. Laser technology has enabled precise manipulation and analysis of molecular structures, facilitating groundbreaking discoveries in chemical reactions, spectroscopy, and materials science.

In environmental applications, lasers are employed for monitoring and mitigating pollution. Laser-induced breakdown spectroscopy (LIBS) enables rapid detection of toxic heavy metals in soil and water, while laser-based remote sensing technologies track greenhouse gas emissions and monitor climate changes. Additionally, lasers are used in environmental remediation, such as laser-induced photodegradation of pollutants and laser-driven wastewater treatment.

Furthermore, laser-driven chemical processes are being explored for sustainable energy production, such as laser-induced ignition of fossil fuels and laser-driven CO<sub>2</sub> conversion. These innovative approaches minimize environmental impact, reduce energy consumption, and promote eco-friendly practices.

The synergy of lasers, chemistry, and environmental science has the potential to transform our understanding of molecular interactions, drive sustainable technologies, and ultimately contribute to a more environmentally conscious future. As research in this field continues to advance, we can expect to see new and innovative applications of laser technology in chemistry and environmental science, leading to a more sustainable and environmentally friendly world.



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## Sharing Best Practices in the Global Chemistry Enterprise

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Many of the key issues facing the future of our planet are global in nature and are intrinsically interconnected, for example, climate change, food shortages, and safe and reliable drinking water. International collaboration and networking provide a useful mechanism to tackle, and potentially overcome, some of these challenges. By their nature, international collaborations encourage and promote diversity and inclusion. Research suggests that diverse groups are much more innovative in solving complex problems than their homogeneous counterparts. This may be due, in part, to the unique local perspective and information that groups with different backgrounds bring to the table. The community of chemists and chemistry-related professionals is truly global. What brings us together is a unity of purpose. To this end, this presentation will focus on four such strategies that educate, inform, and reach out to the community through projects and grants. These specific efforts are Building Opportunity Out of Science and Technology (BOOST), the Global Chemists Code of Ethics (GCCE) effort, the Innovation Corps (I-Corps) programs, and the successful STEM education program called Creative Scientific Inquiry Experiences (CSIE). A description of each type of project will be summarized and the outcomes reported. In addition, a look at water as a global issue, but with local solutions will be presented. The impact on our global chemical enterprise will be discussed in terms of communication trends and in the use of best practices to engage and improve successful careers in both academia and in industry.

## **Vegetable Oil Deodorizer Distillate: An Innovative Capping Agent for Fabrication of the Silver Nanoparticles**

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For the first time, the unsaponifiable part of Vegetable oil deodorizer distillate (USM-VODD) is used as capping and reducing agent for synthesis of silver nanoparticles (AgNPs). Fabricated USM-VODD-derived AgNPs were characterized by Ultraviolet-Visible (UV-Visible) spectroscopy, Fourier Transform Infrared (FT-IR), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM), X-ray Diffractometry (XRD) and Dynamic Light Scattering (DLS). The composition of USM-VODD was evaluated by Gas Chromatography-Mass Spectroscopy (GC-MS). The results showed that the maximum UV absorption of USM-VODD derived AgNPs was observed at 411 nm. According to AFM, the average particle size was  $12.9 \pm 1.2$  nm. USM-VODD functionalized AgNPs were evaluated for the antioxidant and antimicrobial activities. Antioxidant activity of USM-VODD derived AgNPs was determined by the 2, 2-diphenyl-1-picrylhydrazyl (DPPH) method. Both in vitro studies demonstrated the significant potential of USM-VODD derived AgNPs to be used as antioxidant agents. Oxidative stability was also determined by a differential scanning calorimeter (DSC) and it was observed that the oxidative stability of edible oil was substantially increased by the addition of synthesized USM-VODD derived AgNPs, then the synthetic antioxidant i.e., butylated hydroxyl toluene (BHT). Therefore, AgNPs functionalized with USM-VODD have a great potential to be used as natural antioxidant and alternative source of synthetic antioxidants.

## AI-Driven Molecular Spectroscopy for Characterizing Graphene-Metal Oxide Nanocomposites

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Artificial Intelligence (AI) refers to the simulation of human intelligence in machines while characterization of nanomaterials by molecular spectroscopy helps in the deep machine learning. The integration of machine learning with molecular spectroscopy has revolutionized the analysis and application of graphene-based metal oxide nanocomposites. The synergy between molecular spectroscopy and machine learning, highlighting how spectroscopy provides extensive datasets that are used to train machine learning models will be explored. These models, in turn, facilitate advanced analysis, enabling precise characterization and innovative applications of nanocomposites.

Molecular spectroscopy was used in characterization of nanomaterials to develop AI-integrated analysis. While Big Data was collected by different characterization techniques like, Thermogravimetric Analysis (TGA), *Differential Scanning Calorimetry (DSC)* Fourier Transform-Infrared Spectroscopy (FTIR), Particle Size Analyzer (PSA), Powder X-ray Diffraction (XRD), Flame Emission Scanning Electron Microscopy (FESEM), Energy Dispersive X-ray (EDX), High Resolution Transmission Electron Microscopy (HRTEM), Photoluminescence (PL) and Ultraviolet-Visible spectrophotometer (UV-VIS). By using molecular spectroscopy data, machine learning algorithms can identify intricate patterns and relationships within the material properties, leading to improved performance in various applications such as sensors, catalysts, and electronic devices.

Seven Machine Learning (ML) models including Multilayer perceptron (MLP), Support Vector Machine (SVM) Regression, Linear Regression, Random Forest, Additive Regression and K-Nearest Neighbors (KNN) were employed. The models were trained using these ML models and validated using rigorous cross-validation techniques to ensure their generalizability and reliability.

We have successfully synthesized more than 70 nanocomposites with variety of metals and metal oxides nanoparticles including *p*, *d* and *f* block elements along with derivative of graphene. Different synthetic routes have been used while green synthesis is sustainable, environmentally eco-friendly method which helps to eliminate toxic waste. These nanocomposites have been used for their applications in solar cells, solid oxide fuel cells, photocatalytic degradations of pollutants coming out from textile, pharmaceutical, pesticides, and chemical industries.

**Keywords:** artificial intelligence, molecular spectroscopy, graphene, nanocomposites

## **Chemical Analysis of Purslane Leaves Extract Enhanced Humic Acid Coated Nano Particles Properties Against the Multidrug-Resistant Bacteria**

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The biogenic synthesis of NPs by using different plant extracts is common nowadays. The current research was conducted for synthesizing ZnO NPs by green method and humic acid was extracting from coal by IHSS method. Here, *Portulaca oleracea* leaves extract is utilized as an efficient chelating and capping agent for synthesizing ZnO NPs from zinc nitrate hexahydrate salt. The plant ingredients, structure, morphology, thermal behavior, chemical composition and optical properties of ZnO nanoparticles before and after coating were investigated using several characterization techniques XRD, SEM, EDX, BET, ZP, DLS, FT-IR and UV-Vis spectroscopy. The chemical analysis of plant leaf extract verified that this extract is a promising candidate for biosynthesizing ZnO NPs. The synthesized ZnO NPs after coating with humic acid showed more enhanced antibacterial activity on selected gram positive and gram negative bacteria. Thus, coated ZnO NPs might be a good alternative to develop antibacterial agent against the multidrug-resistant bacteria.

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## Computational Chemistry for Next-Generation Drug Discovery: Bridging Innovation and Practical Applications

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Advances in computational chemistry have revolutionized the landscape of medicinal chemistry, offering unprecedented insights into molecular interactions, drug design, and optimization processes. This keynote presentation will explore emerging trends and transformative approaches in computational medicinal chemistry that are shaping the future of drug discovery.

The talk will highlight the integration of in silico techniques to predict molecular behavior, identify promising drug candidates, and reduce the time and cost associated with traditional methods. Case studies will illustrate the practical applications of these technologies in addressing global health challenges, including the design of novel therapeutics for infectious diseases.

Furthermore, the presentation will discuss the critical role of interdisciplinary collaboration in overcoming existing limitations, emphasizing the synergy between experimental and computational approaches. By aligning innovation with practical solutions, computational medicinal chemistry has the potential to redefine the boundaries of what is achievable in modern science.



## Fused Benzothiazino-Quinoline Heterocycles; Synthesis And Mechanistic Study

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2,1-Benzothiazines, hold immense value in medicinal and synthetic organic chemistry due to their wide range of bioactivities and synthetic versatility. The current study focuses on the optimization, synthesis, and characterization of novel benzothiazine fused with quinoline heterocycles and their mechanistic study. A series of novel sultams have been synthesized and characterized using spectroscopic techniques, confirming their chemical structures. These findings highlight the potential of sultam derivatives as valuable scaffolds for future applications in drug discovery and advanced synthetic methodologies. The study demonstrates the isolation of reaction intermediate leading to the design of reaction mechanism.

**Keywords:** Benzothiazine, Sultam, NMR, Mechanism.

## Pure Metal For Electrochemical Water Splitting.

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The primary goal of the study was to create metal electrodes with a high performance characteristic for water splitting using a quick and easy method. This method was then utilized to examine how the substrate and film growth time affected the performance of the electrodes. The electrodes that are created using AACVD (aerosol aided chemical vapor deposition) in a single step and for 30-120 minutes. The photochemical method of splitting water demonstrates an environmentally safe and sustainable way to produce solar hydrogen and oxygen. The materials for the electrodes used in this solar hydrogen method process are semiconductor nanomaterials with a large surface area, good electrical and optical characteristics, and low charge area migration distance. Therefore, the majority of photochemical reactions occur near the electrode's surface. Their physical and chemical characteristics, as well as materials used in photo electrodes, have the power to alter how well a reaction works. Electrochemical water splitting with solar assistance is one of the greatest ways to produce hydrogen, which is then used as a renewable energy source. The primary nature of semiconductor metals has a significant role in regulating the total efficiency of energy conversion. Producing materials for water splitting is difficult because some materials have qualities like stability, charge separation distance, abundance, visible light absorption, and transport. The results of a combination of in situ surface enhancement in a Raman spectroscopy and functional density calculations suggest that there are a number of mechanisms for oxygen evolution on an Au electrode that strongly depend on the voltage of the electrode. The Pd with thin electrocatalyst coating was created using the AACVD technique at a conducting surface. Both XPS and XRD examination revealed a pure metallic phase with Pd deposition. The surface's morphology revealed a highly porous nanostructure with nanoparticles. The presence of mixed metal oxide with iron-based catalysts that have demonstrated great performance in improving oxygen evolution reactions and those that are operating at considerably lower levels. We also looked at how an iron catalyst could perform better by having its surface decorated with platinum or gold to accelerate the evolution of oxygen

and hydrogen during the overall splitting of water. Keywords: H<sub>2</sub> fuel, Electrochemical water splitting, OER, HER, Electrocatalysts, Overpotential, Tafel Slope, Nanocatalysts.

## Revolutionizing Water Splitting: A Quantum Chemical Insight into Single Atom Catalysis

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One of the major environmental problems of the modern day is global warming. Increasing levels of CO<sub>2</sub> in the atmosphere is directly related to the global warming issue. The excessive burning of fossil fuels for energy production and transportation is well accepted in the scientific community to be the leading source of CO<sub>2</sub> emissions. Recently, the use of hydrogen energy has gained interest as it can be a sustainable green source of energy. Production of hydrogen and oxygen gases can be achieved via water electrolysis. we designed a series single atom catalyst (SACs), characterized by the high metal % utilization due to the presence of single catalytic atomic active metal sites, anchored on support materials. The present study investigates the application of late first-row transition metal (TM) doped Mg<sub>12</sub>O<sub>12</sub>, B<sub>12</sub>P<sub>12</sub>, Al<sub>12</sub>P<sub>12</sub>, and late second-row TM dopes B<sub>12</sub>P<sub>12</sub> as single atom catalysts for the cathodic hydrogen evolution reaction (HER) and anodic oxygen evolution reaction (OER). Results from this research showed that the Co@B<sub>12</sub>P<sub>12</sub>, Ni@B<sub>12</sub>P<sub>12</sub>, and Ni@Al<sub>12</sub>P<sub>12</sub> are highly active towards the HER. These SACs showcased  $\Delta G_H$  values that are close to zero, which are -0.20, -0.06, and -0.01 eV, respectively. Their activity was assessed to be superior to a wide range of precious metal based electrocatalysis and competitive to ultra-highly active catalysts. In addition, the Rh@B<sub>12</sub>P<sub>12</sub> revealed bifunctional catalytic activity towards both the HER ( $\Delta G_H = 0.17$ ) and the OER ( $\eta_{OER} = 0.61$  V). This research not only contributes to advancing the green energy field in Bahrain, but also it supports diversifying the country's economy away from fossil fuel-based industries.

## Turning Waste into Solutions: Zn<sub>2</sub>Cr-LDH Derived from Electroplating Effluent for Pyrophosphate Removal

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This study demonstrates the integration of technological advancements into Zn<sub>2</sub>Cr-layered double hydroxide (LDH), synthesized from unused industrial resources, for the effective removal of pyrophosphate (PP) from electroplating wastewater. Emphasizing resource recovery for aquatic environment remediation, Zn<sub>2</sub>Cr-LDH was fabricated via co-precipitation from concentrated metals derived from plating waste, an industrial by-product of metal finishing processes.

Batch experiments were conducted under optimized conditions, including M<sup>2+</sup>/M<sup>3+</sup> ratio, pH, reaction time, and temperature, to assess the material's applicability in water treatment. Comprehensive characterization of Zn<sub>2</sub>Cr-LDH was performed using Brunauer-Emmett-Teller (BET) analysis, X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM/EDS), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS) before and after adsorption.

Optimal conditions (50 mg/L of PP, 1 g/L of adsorbent, pH 6, and 6 hours of reaction) achieved nearly complete PP removal. The primary mechanism for PP adsorption was ion exchange, particularly under acidic conditions. Adsorption followed pseudo-second-order kinetics and conformed to the Langmuir isotherm model, with a maximum adsorption capacity of 79 mg/g. Spent Zn<sub>2</sub>Cr-LDH was successfully regenerated using NaOH with 86% efficiency during the first cycle, and treated effluents met discharge standards (<1 mg/L).

This work underscores the potential of Zn<sub>2</sub>Cr-LDH as a cost-effective adsorbent for wastewater treatment, aligning with national zero-waste policies and advancing circular economy principles through resource recovery.

**Keywords:** Adsorption; Circular economy; Heavy metal removal; Ion exchange; Layer double hydroxide

## **Palladium Anchored Donor Flexible Spectator Ligands as Electrocatalysts for CO<sub>2</sub> Reduction**

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The utilization of CO<sub>2</sub> into synthesis gas as a substitute of processing fossil fuel to produce hydrocarbons is a sustainable and carbon neutral energy technology. The electrochemical reduction of CO<sub>2</sub> into a mixture of CO and H<sub>2</sub> at commercial scale still requires efficient electrocatalyst. In this perspective, a series of new palladium complexes<sup>1-3</sup> with general formulas, [Pd(L<sup>1</sup>)(Y)]Y, [Pd(L<sup>2</sup>)(Y)<sub>2</sub>] and [Pd(L<sup>3</sup>)(Solvento)] Where L<sup>1-3</sup> are different donor flexible spectator ligands and Y/ Solvento are actor ligands, were utilised as active electrocatalysts for the conversion of CO<sub>2</sub> into synthesis gas. All compounds were successfully characterized by various physical methods of analysis such as proton and carbon NMR, FTIR, CHN and single crystal XRD. The redox chemistry of palladium complexes toward carbon dioxide activation suggested an evident CO<sub>2</sub> interaction with each Pd(II) catalyst. The best electrocatalytic activity for CO<sub>2</sub> reduction into synthesis gas under acidic condition of trifluoroacetic acid (TFA) was obtained with a minimum overpotential of 0.11 V, maximum turnover frequency (TOF) of 461 s<sup>-1</sup> and 81% FE of CO. These pincer scaffolds can be stereochemically tuned with its exploration with earth abundant first row transition metals for further improvement in CO<sub>2</sub> reduction chemistry.



## Antimicrobial Activity of Gaozaban(*Onosma Bracteatum*)using pressurized hot Water Extraction

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Plants play a crucial role in human life by serving as a source of maintenance and treatment for numerous diseases affecting both animals and humans. The medicinal plants contain compounds with therapeutic and antibacterial properties that can be employed for the dealing of wide range of diseases brought on by microbial infections. The microbial infections are a major cause of death and depletion. Antibiotic resistance is currently the most prevalent issue, however medications made from medicinal plants are efficient and cost-effective in the fight against the development of resistance. Medical plants are substantial source of antimicrobial agents. Medicinal plant of gaozaban (*Onosma bracteatum*) contains important phytochemicals such as glycosides, phenolics, sugars, tannins, and flavonoids; and is well-known for its effects on mental and cardiovascular issues. The antimicrobial activity of medicinal plant extracts is influenced by factors such as extraction methods and solvent used. The optimization of extraction methods and conditions of the extracted compounds are necessary to ensure the preservation and enhancement of antimicrobial activity in plant extracts using green extraction methods. Green extraction methods, which focus on minimizing environmental impact and maximizing sustainability, have an impact on the biological action of extracts derived from plants. These methods aim to reduce the use of harmful solvents and energy-intensive processes typically associated with traditional extraction techniques. Green extraction methods, such as pressurized hot water extraction (PHWE), utilize water as a solvent or co-solvent, reducing or eliminating the need for harmful organic solvents. This reduction in solvent residues can enhance the safety of the plant extracts and their antimicrobial activity. The current study aims to prepare the extract derived from gaozaban (*Onosma bracteatum*) by using pressurized hot water extraction (PHWE) and to evaluate the antimicrobial activity of *Onosma bracteatum* extract by agar well diffusion method. In this research work, the plant material of gaozaban (*Onosma bracteatum*) was collected, washed and shade dried. The dried-up plant material of gaozaban was grinded in to finely ground powder by grinder. The pressurized hot water extract was prepared

by the utilization of espresso machine. The dried and finely ground powder of plant material was firmly packed into portafilter (sample compartment) of espresso machine. The water reservoir of espresso machine was filled with 500ml of distilled water. The pressurized hot distilled water was passed through the finely ground plant material. The volume of extract was collected and, then cooled in an ice bath. The extract obtained from espresso machine was filtered and concentrated by removing solvent. the concentrated extract was evaporated to dryness in oven. The 50mg/ml, 100mg/ml and 150mg/ml stock solutions of extract were prepared in double deionized water. The anti-bacterial properties of extract were evaluated by agar well diffusion method against sea bacteria (SW3-5b) and (SW2-5/1). The results showed that plant extract of *Onosma bracteatum* revealed the bacteriostatic action on the sea water bacterial strains (SW3-5b) and (SW2-5/1). The extract concentrations of 150mg/ml have significant bacteriostatic activity against sea water bacterial strain (SW3-5b) over the area of 16mm. While extract concentrations of 50mg/ml and 100mg/ml also showed bacteriostatic action on the sea water bacterial strain (SW3-5b) over the area of 6mm and 10mm respectively. The extract concentrations of 50mg/ml and 100mg/ml had also shown the bacteriostatic activity against sea water bacterial strain (SW2-5/1) over the areas of 6mm and 12mm respectively. The phytochemical screening of pressurized hot water extract of *Onosma bracteatum* was carried out by performing standard tests that revealed the presence of tannin, saponin and phenolic compounds; and absence of alkaloid, flavonoid, glycoside and terpenoid. It concludes that the aqueous extract of *Onosma bracteatum* obtained through pressurized hot water extraction have bacteriostatic activity. In future, the extract of gaozaban (*Onosma bracteatum*) obtained through pressurized hot water extraction need to be inspected for further isolation and characterization of phytochemicals.

## Iridium-Catalyzed Aromatic C-H Activation/Borylation

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Functionalized aromatic hydrocarbons have applications in wide range of areas including pharmaceuticals, agrochemicals, polymers, catalysis, and organic electronic materials etc. Functionalization of aromatic hydrocarbons was discovered by Michael Faraday in 1826 when he showed that benzene and nitric acid react together to produce nitrobenzene. Over the past couple centuries, the organic synthetic chemists have utilized electrophilic & nucleophilic aromatic substitutions, as well as directed *ortho* metalation approaches as the main routes for the preparation of functionalized aromatics. Despite some good reactivity patterns governed by electronic factors yielding high regioselectivities, these methodologies do have certain limitations, especially when regioselectivities not observed in these methodologies are desired. As a consequence, long-protracted routes have often been required to prepare very simple aromatic compounds. In order to solve these problems, new reactivity patterns with unique regioselectivities, complementary to the existing ones, are desired.

Iridium-catalyzed aromatic C-H activation/borylation has emerged as an alternative and convenient methodology for the regioselective functionalization of aromatic/heteroaromatic hydrocarbons. The most striking feature of this new tool available to the synthetic chemist is that the regioselectivities are governed by sterics, and hence, these are complementary to those found in electrophilic aromatic substitution or directed *ortho* metalation. This unique feature has allowed the preparation of new aromatic building blocks, which were previously either unknown or difficult to synthesize. In the present talk we will discuss the applications of this new synthetic methodology for the preparation of new fluorinated (hetero)aromatic building blocks.

## Ag@ZIF-8 Composite for Removal of Ciprofloxacin

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Ag@ZIF-8 was successfully prepared by using a facile and fast method of hydrothermal synthesis at room temperature and characterized by a variety of techniques. Results indicate that prepared Ag@ZIF-8 contains a very beautiful morphology with a great active specific surface area than solo ZIF-8. The prepared Ag@ZIF-8 contains a greater pore size. The adsorption performance of Ag@ZIF-8 was further studied with the removal of ciprofloxacin from polluted water as its concentration increased in water from the waste products due to being prescribed globally to treat patients. Various adsorption parameters, such as contact time, pH, and initial concentrations of medicine and composite, were optimized. The kinetics parameters of the adsorption process were determined by applying the pseudo first-order kinetic model (PFO) and pseudo second-order (PSO) kinetic model. Ciprofloxacin showed chemical adsorption as it followed PSO kinetics. In the case of medicine, adsorption isotherm data matched well with Freundlich as compared to Langmuir model which revealed the multilayer adsorption of pollutant. Ag@ZIF-8 was found to be an efficient adsorbent for the adsorption of ciprofloxacin, having maximum 130 mg/g adsorption capacity.

**Keywords:** ZIF-8, MOFs, Ag@ZIF-8 composite, Water purification, Adsorption.

## Exceptionally Large Nonlinear Optical Response of Rationally Designed Alkaline Earthides

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Design of new and efficient nonlinear optical (NLO) materials is the subject of immense scientific investigation in the recent times because of their potential applications in photonics, dynamic imaging, data storage, optical signal processing devices and computer devices. Several strategies are proposed to design materials with remarkable nonlinear optical response. An effective strategy is to introduce excess electrons in a system either in the form of electrides, alkalides, alkaline earthides or diffuse excess electrons. In this presentation, design principle, linear and nonlinear optical properties of alkaline earthides by doping of alkali and alkaline metals on a variety of complexants will be presented. The alkaline earthides designed here possess remarkably high nonlinear optical response where hyperpolarizability reaches up to  $1 \times 10^8$  au, comparable to the best value reported in the literature. The remarkable NLO response is attributed to partially polarized p electrons which are quite different than polarized s electrons of alkali metals in alkalides.

## Improving Mechanical and Thermal Resilience in Selected Thermoplastic Polymeric Matrices

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The class of polymers, thermoplastic elastomers exhibit flexibility, good manufacturing potential and heat treatment. The macromolecules' high processability makes them suitable in a wide range of fields, however in terms of material attributes; mechanical strength and thermal stability remain to be developed. A great more attention has been devoted towards the fabrication of nanocomposites with additives of high strength. The properties described above have been strengthened by ensuring their adaptability. The insulating polymer matrix has been given conductivity via PPy grafting of SEBS and fabricating nanocomposites employing organically modified montmorillonite (OMMT) and CNTs as reinforcement. Through PPy grafting at SEBS and nanocomposites formation using OMMT and CNTs as reinforcement, conductivity has been introduced in to the insulating polymer matrix. Tensile properties of the material have also been studied and reported for SEBS-g-MA/OMMT which resulted in improved mechanical strength. The nanocomposites have been characterized using fourier transform infrared spectroscopy (FTIR), nuclear magnetic resonance (NMR), X ray Diffraction (XRD), thermogravimetric analysis (TGA), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and tensile testing. The presentation's key emphasis will be on the author's work in improving elastomers' mechanical strength while maintaining their elastic and processable potentials.

**Key Words:** Flexibility, Fabrication, Reinforcement, Conductivity, Mechanical Strength

## Upcycling of Industrial Waste for Sustainable Development and Circular Economy

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Fly ash as a particulate and leachate pollutant has been recognized as human carcinogen. It is a key player of smog and climate change. Its dumping can be detrimental for soil fertility and ground water as well as financial liability. The most attractive and sustainable mitigation of fly ash waste is its recycling for value addition materials. Synthesis of fly ash-based zeolites as value-added material is an economical and sustainable approach. In this work a variety of fly ashes from boiler plants of different industries were used for the synthesis of fly ash based active zeolites. Different fly ash based zeolites and zeolite synergized photo-catalysts prepared by conventional and advanced curing techniques were characterized by state-of-the-art analytical techniques like; XRD, SEM, FTIR, ICP-OES and CEC and investigated for their wastewater treatment potential, Keeping in view the findings of this study, it is very reasonable to conclude that recycling of fly ash waste for wastewater treatment is a positive move towards achieving a healthy environment and green technology.

**Keywords** Fly ash, Smog, Synthesis, Zeolites, Water treatment

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## Advancing Materials Discovery & Applications through Computational Chemistry

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Computational chemistry is the branch of chemistry that employs the use of computer modeling to solve chemical problems. Computational chemistry has emerged as a reliable tool for the investigation of geometric, electronic, and optical properties of molecular systems and to study the origin of various chemical phenomena. The Computational Chemistry Group at COMSATS University Islamabad, Lahore Campus, employs cutting-edge theoretical and computational techniques to explore and design innovative materials for a wide range of applications. Our research encompasses the prediction and characterization of materials for nonlinear optics, drug delivery systems, chemical and biosensors, separation membranes, and beyond. By integrating quantum chemical calculations, molecular dynamics simulations, and data-driven modeling approaches, we aim to provide fundamental insights and accelerate the development of functional materials. This presentation will highlight our group's key research directions, recent achievements, and collaborative opportunities, showcasing how computational chemistry serves as a powerful tool in modern materials science.

**Keywords:** Simulations; Experimental; DFT



## Sustainable Hydrogen Peroxide Synthesis Using Bismuth-Modified Biochar

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This study presents the development of a novel, renewable biochar-based electrode material for the sustainable electrochemical synthesis of hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) via oxygen reduction. Biochar was derived from waste Himalayan poplar wood (*Populus ciliata*) through pyrolysis at 1000°C. The resulting biochar was characterized using scanning electron microscopy (SEM) to examine its morphology, X-ray diffraction (XRD) to analyze its crystal structure and degree of graphitization, and Raman spectroscopy to probe its internal structure. The characterization confirmed that the biochar possessed a highly porous structure with both ordered and disordered carbon frameworks. The biochar was further modified by ball milling with bismuth carbonate and annealing at 600°C to produce bismuth-doped biochar. XRD analysis confirmed the successful incorporation of bismuth into the carbon framework. Electrochemical impedance spectroscopy (EIS) revealed that the bismuth-doped biochar exhibited lower equivalent series resistance compared to pristine biochar. The bismuth-doped biochar demonstrated higher current density than the undoped biochar. Additionally, the bismuth-doped biochar showed enhanced selectivity for hydrogen peroxide production compared to pristine biochar. These findings highlight the potential of utilizing biowaste to develop eco-friendly electrode materials for the on-site, on-demand synthesis of hydrogen peroxide, offering a sustainable alternative for industrial applications.

**Keywords:** Biochar, Pyrolysis, Bismuth Doping, Hydrogen Peroxide, Sustainable Electrode, Renewable Materials.

## Biosynthesis of Polyhydroxy Butyrate using Agricultural By-Products Through Solid State Fermentation

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The conventional non-biodegradable plastic is made up of polyethylene and is one of the major causes of environmental pollution. The biodegradable plastic, polyhydroxybutyrate (PHB), serves as an alternate and have number of industrial and medical applications. Main hurdle in commercialization is cost of substrate as 3 tons of glucose is required for production of one ton of PHB. Hence, the study was conducted to check the potential of various sugar rich agricultural by-products (rice polishings, wheat bran and corn cob) for the manufacturing of PHB using the technology of solid-state fermentation by *Bacillus thuringiensis*. The optimization studies were conducted using one factor at a time approach for hyper-production of PHB. The maximum amount of bioplastic (420 mg/100g) was gained by fermenting rice polishing for 72 hours at substrate water ratio of 10:36 and addition of 1 ml inoculum. The yield further improved by setting temperature at 300°C and pH at 7. By addition of 2% NaCl, 2% MgSO<sub>4</sub> and 1.5% of KH<sub>2</sub>PO<sub>4</sub>.2H<sub>2</sub>O, and among nitrogen sources, 1% corn steep liquor and 0.75% urea, yield of PHB was improved to 680 mg/100g. For functional groups identification FTIR analysis was performed in comparison to the standard. PHB was found to be 98% pure by spectrophotometric studies. The results indicates that agricultural by-products can serve as cheap substrate for bioplastic synthesis. The optimized conditions will be helpful for commercial manufacturing of the biopolymer.

**Key words:** Agricultural by-products, Polyhydroxybutyrate, solid state fermentation, *Bacillus thuringiensis*.

## Macrolides resistance of ermB gene in *Streptococcus uberis* associated with bovine mastitis and improvising the molecular docking as an alternate treatment

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Sub-clinical bovine mastitis is an intramammary infection and *Streptococcus uberis* is responsible for lactation insufficiency. Macrolides are provided as mastitis medication, but this train ascribes antibiotic resistance. *Streptococcus uberis* was isolated from 10 sub-clinical and 10 clinical milk samples of mastitic cows by inoculated on 5% sheep blood agar at 37°C for 48 hours. Antimicrobial resistance activity of *Streptococcus uberis* against erythromycin, azithromycin was identified by the disc diffusion method on Muller Hinton agar and molecular identification ermB was performed using sequencing. For alternate treatment against bovine mastitis, in-silico was improvised. Molecular docking was performed on the sequence obtained as a result of in-vitro approach with phytochemicals. Chi-square and Fisher's exact test was performed for the statistical analysis. Antimicrobial resistance activity of *Streptococcus uberis* against macrolide was identified that reduces the use of erythromycin, azithromycin as medication against *S.uberis*. Macrolide resistance was facilitated by the ermB and mefA genes. In-silico approach provided the effective phytochemical for the treatment of bovine mastitis.

**Keywords:** *Streptococcus uberis*, bovine mastitis, macrolide resistance, in-silico molecular docking

## Engineering Metal-Doped Tungsten Oxide Nanocomposites: Synthesis and Applications

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Pure  $\text{WO}_3$  NPs and (Cu, Mo) co-doped  $\text{WO}_3$  NCs were synthesized using the hydrothermal method. A set of (Cu, Mo) co-doped  $\text{WO}_3$  NCs doped at different concentrations of 2%, 4%, 6%, 8% and 10% mol were successfully prepared. These NCs were evaluated for their photocatalytic performance in degrading methylene blue (MB) under sunlight evaluated by UV-Vis spectroscopy. Among the synthesized samples, the highest photocatalytic efficiency was present in the 10% (Cu, Mo) co doped  $\text{WO}_3$  NCs. In addition, sulfur doped graphitic carbon nitride (S-g $\text{C}_3\text{N}_4$ ) was synthesized from thiourea thermal decomposition, which had the potential as an efficient photocatalyst. In the aim of improving photocatalytic activity, several (Cu, Mo) co doped  $\text{WO}_3$ / S-g $\text{C}_3\text{N}_4$  nanocomposites (NCs) were synthesized by mixing 10% (Cu, Mo) co doped  $\text{WO}_3$  NC with S-g $\text{C}_3\text{N}_4$  at 10%, 30%, 50%, 70%, and 90%. Structural, morphological, optical, and other properties of the synthesized and NPs, NCs were systematically characterized. UV-Vis spectroscopy was used to measure their photocatalytic performance and demonstrate their potential for environmental remediation.

## **Mentha piperita Essential Oil Mediated Synthesis of Fe<sub>3</sub>O<sub>4</sub>/La<sub>2</sub>O<sub>3</sub>/GO Nanocomposite and its Chemical and Biological Applications**

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In this paper, current study investigated the synthesis, characterization, and applications of iron oxide (Fe<sub>3</sub>O<sub>4</sub>) and lanthanum oxide (La<sub>2</sub>O<sub>3</sub>) nanocomposites integrated with graphene oxide (GO) and reduced graphene oxide (rGO) by using eco-friendly methods. A combination of sol-gel and one-pot synthesis techniques utilized Mentha piperita essential oil to synthesize the reduced graphene oxide by green reduction method. Spectroscopic characterization such as X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), UV-visible, and Fourier transform infrared (FTIR) spectroscopy were applied and their results confirmed the successful integration of GO and rGO with Fe<sub>3</sub>O<sub>4</sub>/La<sub>2</sub>O<sub>3</sub>, highlighting distinct crystallographic phases and uniform nanoparticle dispersion. The photocatalytic efficiency of Fe<sub>3</sub>O<sub>4</sub>/La<sub>2</sub>O<sub>3</sub>/rGO composites was notable, achieving up to 97% degradation of methylene blue due to enhanced electron-hole pair separation and superior rGO adsorption capacity. Additionally, significant antibacterial activity against E. coli, S. aureus, and P. aeruginosa was observed, with Fe<sub>3</sub>O<sub>4</sub>/La<sub>2</sub>O<sub>3</sub> nanoparticles surpassing GO and rGO in efficacy. This research demonstrates the potential of Fe<sub>3</sub>O<sub>4</sub>/La<sub>2</sub>O<sub>3</sub>/rGO composites for effective environmental remediation and antibacterial applications.

## Microbial Systems as Mimics for *in vivo* Drug Metabolism

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Drugs, taken through various means, undergo extensive metabolism upon interaction with the body enzyme system, leading to the formation of variety of metabolites. Identification and characterization of these metabolites is of utmost importance to know about the possible effects they might have on the body. Over the past few decades, microbial biotransformation has developed as a technique for structural modification of organic compounds, employing the microbial enzyme systems. Biotransformation of marketed drugs, in most cases, has led to the synthesis of products, already identified as *in vivo* metabolites of the same drug. Thus, the technique can be used effectively for the biotransformation of bioactive compounds or possible lead molecules. This would provide an overview of the probable metabolic pathway and metabolites, possibly produced inside the body, upon ingestion. In this context, microbial transformation of several steroidal drugs was carried out, leading to the formation of products, some of which have already been identified as *in vivo* metabolites, making these microbial strains potential models for *in vivo* metabolism of drugs.

## Highly Efficient CoS/S@g-C<sub>3</sub>N<sub>4</sub> Nano Composite for Degradation of Pollutants in Wastewater

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This research work synthesized CoS/S@g-C<sub>3</sub>N<sub>4</sub> nano Composites to address the issues water pollution problem. Prepared composite was used to remove methylene blue which is major organic pollutant. It was doped with sulphur doped graphitic Carbon nitride, resulting in the desired Nano Composites. Nano Composites were observed and characterized with the help of FTIR, while the photocatalytic activity was observed determined with use of a UV-visible spectrophotometer. The decrease in absorbance was an indicator of photocatalytic activity due to the decline in concentration of methylene blue. 90% CoS/S@g-C<sub>3</sub>N<sub>4</sub> nanocomposite had the efficiency i.e. 93%.

## Dual doped ZnO Nanomaterials: An effective Catalyst for Environmental Remediation

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This study adopted the sol-gel process to create ZnO nanomaterials doped with Fe and La i.e., Zn<sub>0.95-x</sub>Fe<sub>0.05</sub>La<sub>x</sub>O (x = 0, 0.01, 0.04, 0.07, 0.10). The synthesized materials were analyzed using PXRD, UV-Vis, FESEM, EDX, and VSM. UV-Vis spectroscopy demonstrated a reduction in the band gap with the increased concentration of doping materials, ranging from 3.02 eV for pristine ZnO to 2.559 eV for the ZnO nanomaterials with the highest dopant concentration. VSM investigation demonstrated room-temperature ferromagnetic behavior, with the Zn<sub>0.85</sub>Fe<sub>0.05</sub>La<sub>0.10</sub> sample exhibiting the maximum saturation magnetization (0.0240 emu/g) and retentivity (0.00037 emu/g). According to this study, due to the synergistic effect of Fe and La doping, the photocatalytic activity of dual-doped ZnO materials for methylene blue degradation under sunlight has been greatly improved, reaching an efficiency of up to 82.46% at pH 12 with a catalyst dosage of 30 mg. Even after five cycles, the material maintained 71.5% efficiency demonstrating good reusability. This work demonstrates that these materials can be utilized as effective photo catalyst for environmental remediation.

**Keywords:** Photocatalyst, dual doped, nanomaterials, pollutants



## **Fabrication of Cd Doped Cr<sub>2</sub>O<sub>3</sub> Composite with S-g-C<sub>3</sub>N<sub>4</sub> as Efficient Electrocatalyst for Overall Water Splitting**

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The creation of green and sustainable energy sources is major research focus now adays due to the growing demand for energy worldwide and environmental concerns. This research introduces a method for producing hydrogen efficiently using electrochemical water splitting with nanoparticles. A clean fuel substitute with a high energy density is hydrogen. To increase electrochemical water-splitting activity, a bifunctional catalyst is needed to catalyze HER (Hydrogen evolution reaction) and OER (Oxygen evolution reaction). In this project Chromium oxide (Cr<sub>2</sub>O<sub>3</sub>) nanoparticles, a series of cadmium-doped Cr<sub>2</sub>O<sub>3</sub> by varying weight percentage of Cd (1,3,5,7 and 9 wt. %), and a composite of 9% Cd-doped Cr<sub>2</sub>O<sub>3</sub> on sulfur-doped graphitic carbon nitride (Cd. Cr<sub>2</sub>O<sub>3</sub>@SGCN) of varying weight percentage of SGCN (10, 30, 50, 70, and 90 wt. %) were all prepared using an environmentally friendly one-pot hydrothermal process. FTOs are used as working electrodes, modified with nanoparticles and perform experiments like CV, LSV and EIS to check their activities for OER and HER. By comparing the results of all the catalysts, we will get to conclude that 50% Cd. Cr<sub>2</sub>O<sub>3</sub>@ SGCN shows highest activity compared to all other different types of nanomaterials tested.

## Postbiotics and Their Role in Gut Health and Immunity: Mechanisms, Benefits, and Future Research

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Postbiotics, bioactive compounds derived from probiotic fermentation, have garnered significant attention for their potential role in gut health and immune regulation. Unlike probiotics, postbiotics do not require live microorganisms to confer benefits, making them a stable and promising alternative for improving host health. This systematic review synthesizes peer-reviewed studies published between 2015 and 2025, examining the mechanisms, health benefits, and clinical applications of postbiotics. Key components, including short-chain fatty acids (SCFAs) such as butyrate, peptides, exopolysaccharides, and enzymes, contribute to gut microbiota modulation by enhancing intestinal barrier integrity, reducing inflammation, exerting antioxidant effects, and maintaining microbial balance. For instance, *Faecalibacterium prausnitzii* produces butyrate, which supports gut barrier function and exhibits anti-inflammatory properties. Additionally, postbiotics play a crucial role in immune regulation by modulating cytokine production, enhancing regulatory T cell activity, and balancing pro- and anti-inflammatory pathways, thereby contributing to immune homeostasis. Clinically, postbiotics show promise in managing gastrointestinal disorders, allergies, and immune-related diseases. Despite these benefits, knowledge gaps remain regarding optimal dosing, long-term safety, and precise mechanisms of action. Future research should focus on large-scale clinical trials, standardized formulations, and elucidating molecular pathways to maximize their therapeutic potential. This review underscores the emerging role of postbiotics as a viable strategy for enhancing gut and immune health while highlighting key areas for further investigation.

**Keywords:** Postbiotics, Gut Health, Immune Health, Nutritional Biochemistry, Bioactive Compounds.

## Eco-Friendly Bimetallic Ionic Liquids as Dual-Function Extractants and Catalysts for Efficient Oxidative Desulfurization of Fuels

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A series of dicationic ionic liquids (DcILs) with varying alkyl chain lengths and  $[\text{FeCl}_2, \text{fBr}]^+ \text{Br}^-$  as the counter anion were synthesized and comprehensively characterized using FT-IR, Raman spectroscopy, mass spectrometry, and single-crystal X-ray analysis. Their thermal stability, chemical structure, and elemental composition were further analyzed through thermogravimetric analysis (TGA) and X-ray photoelectron spectroscopy (XPS). These DcILs were explored as both extractants and catalysts for oxidative desulfurization (ODS) of liquid fuels, employing  $\text{H}_2\text{O}_2$  as an oxidant. Key reaction parameters including reaction time, temperature, catalyst loading, oxidant-to-sulfur ratio, and sulfur substrate reactivity were systematically evaluated. The DcILs demonstrated high extraction and catalytic efficiency under mild conditions, achieving rapid reaction equilibrium and significant sulfur removal at room temperature with minimal catalyst and oxidant consumption. Due to their low solubility in liquid fuels and high recyclability, these DcILs present a green and eco-friendly approach to desulfurization, minimizing fuel contamination while enhancing sustainability.

**Keywords:** Design, Synthesis and Structural Studies

## **Computational Analysis Of Interactions Between Related Transcription Factors And Wheat Derived miRNA Against WYMV**

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Wheat yellow mosaic virus (WYMV) is a major pathogen affecting wheat (*Triticum aestivum* L.), causing severe yield losses. Growth-Regulating Factors (GRFs), a class of transcription factors, play crucial roles in plant growth, development, and stress responses, including viral resistance. In this study, an in-silico approach was employed to investigate miRNA-mediated post-transcriptional regulation of GRF genes in wheat to elucidate potential mechanisms conferring resistance to WYMV. We retrieved wheat GRF gene sequences and performed miRNA target prediction using bioinformatics tools such as RNA hybrid. High-confidence miRNA binding sites within the 3' UTR regions of GRF genes were identified based on minimum free energy (MFE) values, with a threshold of -0.7 kcal/mol. Among the predicted interactions, stress-associated miRNAs such as miRNA-8726 exhibited strong binding affinities (-2.5 kcal/mol), suggesting potential regulatory roles in WYMV response pathways. To visualize the regulatory landscape, an interaction network was constructed using Python-based NetworkX, mapping miRNA-GRF interactions. The network analysis revealed key miRNAs that target multiple GRF genes, suggesting a complex regulatory system underlying wheat's defense against viral infection. This study provides valuable insights into the molecular interplay between miRNAs and GRF genes, highlighting candidate miRNAs for further experimental validation and potential use in genetic improvement strategies to enhance WYMV resistance in wheat.

## **Decoding Nutrient Transport: *In-Silico* Optimization of OsMRS2-2 for Magnesium-Enriched Rice**

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Magnesium is an essential nutrient for supporting muscle function, nerve signaling, energy production, and mediates over 300 enzymatic reactions vital for general human health. In plant growth, it plays a critical role in chlorophyll synthesis, enzyme activation, and nutrient transport. This study focuses on enhancing Mg uptake in rice (*Oryza sativa*) by targeting the OsMRS2-2 transporter gene, primarily expressed in roots, to improve both plant health and nutritional value of rice. By upregulating OsMRS2-2, we aim to increase Mg absorption from the soil, addressing both dietary deficiencies in consumers and Mg scarcity within the plant itself. To achieve this, the upstream regulatory sequence of OsMRS2-2 was retrieved from Gramene and analyzed for key regulatory motifs using PlantCARE. Transcription factors and their binding sites were identified through PlantRegMap to determine regulatory interactions. Guide RNAs (gRNAs) were designed via CRISPOR for precise genome editing, with selection criteria based on efficiency and target site specificity. Homology arms for knock-in modifications were designed using Benchling, followed by homology-directed repair (HDR) simulations to evaluate editing efficiency. Beyond improving Mg uptake, this study provides insights into the role of transcription factors and their binding motifs in regulating stress-related genes, offering a broader perspective on plant resilience and biofortification strategies.

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## **Biofuel and its Importance in the Future**

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As global energy demands continue to rise due to rapid population growth and industrialization, the depletion of non-renewable fossil fuels and their adverse environmental impacts have become critical concerns. The extraction, refining, and combustion of fossil fuels contribute significantly to pollution, land degradation, and greenhouse gas emissions, which accelerate climate change. In response to these challenges, biofuels have emerged as a promising alternative energy source that offers sustainability, reduced carbon emissions, and efficient utilization of organic waste. By converting biomass into fuel, biofuels not only address energy shortages but also contribute to environmental conservation by reducing dependence on finite fossil fuel reserves. One of the primary advantages of biofuels is their ability to reduce greenhouse gas emissions. Unlike fossil fuels, which release carbon stored underground for millions of years, biofuels operate within a shorter carbon cycle, significantly lowering net carbon emissions. Additionally, biofuels help in waste management by converting organic waste into energy, thereby reducing landfill accumulation and pollution. They also provide economic benefits by creating job opportunities in agriculture, research, and biofuel production, fostering economic growth and energy security in both developed and developing nations. Despite their numerous benefits, biofuels face several challenges that must be addressed for large-scale adoption. High production costs, land and water requirements, and the energy-intensive nature of some biofuel refining processes can limit their efficiency and affordability. As the world transitions towards cleaner and more sustainable energy solutions, biofuels will play a crucial role in reducing dependence on fossil fuels and mitigating climate change. With continuous advancements in biofuel technology, along with policy support and public awareness, biofuels can serve as a viable, long-term energy solution. By integrating biofuels into the global energy mix, we can move towards a more sustainable and environmentally responsible future, ensuring energy security for generations to come.

## The Microbiome and Mental Health: Unlocking Novel Therapies for Depression and Anxiety

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Depression and anxiety are the most prevalent mood disorders which are affecting mental health of people globally nowadays. Gut-brain axis, which is the bidirectional communication between the gut microbiota and the central nervous system of brain mainly via the biochemical signaling of vagus nerve, plays a pivotal role in regulation of mental health and behavior. This new paradigm to mental health incentivizes biotechnologists to understand and study the gut microbiota in an individual who is non-anxious and happy, and then compare it to the one present in an anxious and depressed person. High throughput rRNA gene sequencing of gut microbiota is performed by taking sample from gut. Emerging studies show that dysbiosis (imbalance of gut microbiota) shapes mental health and causes symptoms of anxiety and depression in individuals. Certain gut bacteria produce cytokines which influence brain processes and behavior of a person. Short chain fatty acids and specific bacterial species regulate mood by modulating neurotransmitters like serotonin, dopamine, GABA. Probiotics, prebiotics and psychobiotics improve gut-brain axis. Probiotics intake balance beneficial bacteria of gut microbiota like Bifido-bacterium and Lactobacillus rhamnosus. These bacteria reduce gut inflammation and alleviate mood disorders. Fecal microbiota transplantation (FMT) in animals reduce anxiety and depression while in humans it is still understudied. Research in the domain of microbiome-based therapies has been an exciting piece of work. Exploring the potential of microbiome-based therapies offers a promising avenue for our mental wellness in relation with the balance of gut microbiota.

## **Gene Editing Strategies to Extend Banana Shelf Life: Combating Browning for Improved Post-Harvest Stability**

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Banana is the fourth largest fruit crop with over 153 million tons production annually and over 400 million people feed on it. Its short shelf life makes it a debatable problem for farmers and stores. The main issue is its browning attributable to any damage, or whenever it is peeled. Moreover, there are some phenolic compounds such as catechins, chlorogenic acid present which are acted upon by some enzymes and converted into quinones when any accident happens to its covering. Various researchers in UK based Biotech Company focused on the browning of the banana and successfully developed a GMO banana which lasts for more than 12 hours after peeling. It was first sold in Philippine and got a good marketing response. The scientists did not introduce any foreign gene rather they made some modification in banana's own genome. A gene present in banana called MaACO1 produces polyphenol oxidase (PPO) which mainly cause the browning of it. RNA interference (RNAi) implemented by the scientists to silence the gene which is causing it, and it has a high future potential in preventing food spoilage. Furthermore, scientists stated that the experiments on refined gene editing techniques can improve shelf life of bananas. In this way, it can remain fresh for days instead of hours. Eventually, the non-browning bananas have a promising future in enhancing food security and may also add to successful marketing of the product by attracting buyers.



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## **Revolutionizing Pain Relief: The Power of Gene Therapy**

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Chronic pain due to various reasons affects millions of people worldwide and coping with pain is the most anticipated solution for long-lasting pain management in the society. According to World Health Organization, 22% global population experience chronic pain. It can be caused by a disease or by any damage or injury to bodily tissues which may last for 6 months or beyond. Paracetamol and many other anti-inflammatory drugs have been used as a standard treatment to relief pain but failed to determine the underlying cause of the disease. However, scientists have stated that gene therapy is the most accurate and precise technique in targeting the pain pathways. Furthermore, the pharmaceutical and biotech industries have been focusing on nature, developing drugs from biological components, i.e., oligonucleotides (DNA), enzymes, proteins rather than using chemically modified medicines. Emerging studies show that gene therapy including CRISPR(Clustered regularly interspaced short palindromic repeats), small interfering RNAs, and antisense oligonucleotides are effective in gene editing, as they target primary and sensory neuron and non-neurological cells, i.e., glia and chondrocytes. These advancements have helped patients in believing that incurable and inherited diseases can be treated. 20 gene therapy products have already been introduced in the Biotech industries and over 2000 human gene therapy clinical trials have been reported which made gene therapy commercially profitable. The development of new delivery tools for performing gene therapy are being highly considered by the scientists and it will be efficacious in this area of pain management.

## **Microbiome and Immunity**

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The human microbiome, a complex community of microorganisms inhabiting various body sites, plays a pivotal role in shaping and modulating the immune system. This symbiotic relationship begins at birth and evolves throughout life, influencing immune development, pathogen defense, and systemic homeostasis. Key microbiomes, including those in the gut, skin, oral cavity, respiratory tract, and urogenital system, contribute uniquely to immune regulation. The gut microbiome, the most diverse, is central to immune function through the production of short-chain fatty acids (SCFAs) like butyrate, which strengthen epithelial barriers, promote regulatory T cell (Treg) differentiation, and suppress inflammation. Similarly, the skin and oral microbiomes protect against pathogens by maintaining microbial balance and producing antimicrobial compounds. Disruption of this equilibrium, termed dysbiosis, is linked to immune dysregulation, contributing to autoimmune diseases, inflammatory conditions, and increased infection susceptibility. Dysbiosis mechanisms include impaired barrier integrity ("leaky gut"), and reduced anti-inflammatory metabolite production. The microbiome immune axis involves commensal microbes train innate and adaptive immunity by enhancing antimicrobial peptide production, antigen presentation, and immunological memory, while the immune system regulates microbial composition through IgA secretion and inflammatory responses. Therapeutic strategies, such as probiotics, prebiotics, and aim to restore microbial balance, demonstrating efficacy in treating *Clostridioides difficile* infections and modulating chronic inflammatory diseases. Emerging approaches, including engineered microbes and personalized microbiome profiling, highlight the potential for precision medicine. However, challenges like antibiotic resistance, offering novel avenues for disease prevention and treatment. Future research must address the complexities of host microbe interactions, optimize therapeutic interventions, and ensure equitable access to microbiome-based therapies to harness their full potential in promoting human health.

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## **Revolutionizing Cancer Treatment: The Power of Immunotherapy**

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Cancer immunotherapy has revolutionized oncology by leveraging the body's immune system to target and eliminate malignant cells. Unlike traditional treatments such as chemotherapy and radiation, immunotherapy offers a more precise and durable approach with fewer systemic side effects. This presentation explores principles of cancer immunotherapy and key immunotherapeutic strategies, including immune checkpoint inhibitors, CAR-T cell therapy, cancer vaccines, and monoclonal antibodies. We will discuss their mechanisms of action, current clinical applications, and emerging research trends along with case studies and real-world impact. Additionally, we will address challenges such as immune resistance and adverse effects, highlighting ongoing efforts to optimize treatment efficacy. By understanding the advancements in cancer immunotherapy, we move closer to personalized and curative solutions for various malignancies.

## Design of Polysaccharide-Based Photocurable Hydrogels for Wound Repair Applications

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Hydrogel is the most appropriate biomaterial for wound healing applications due to its correspondence with the extracellular matrix (ECM) and can maintain a moist environment, facilitating the healing process. However, the development of a hydrogel possessing significant characteristics such as suitable mechanical strength, adhesiveness, antibacterial activity and biocompatibility remains a limitation. Here, polysaccharide-based photocurable hydrogels were synthesized through UV crosslinking and their properties were analyzed by FTIR, rheology, adhesion test, antibacterial activity and biocompatibility assays. FTIR analysis confirmed the interactions among the polymers present in the hydrogel network. The rheological studies revealed that UV crosslinking increased the mechanical strength of these hydrogels. The prepared hydrogels demonstrated enhanced adhesive strength and inhibited the growth of bacterial strains i.e., *E. coli* and *S. aureus*, evaluated through inhibition zone method. Biocompatibility assays are important to evaluate the hydrogels' potential for tissue regeneration. The findings suggested that the prepared hydrogels promoted the viability and growth of cells. These results represented that the designed hydrogels may be employed in wound healing applications.

**Keywords:** polysaccharide; photocurable; hydrogel; wound repair.

## **Decoding Immunological Aging: from Molecular Decline to Targeted Interventions**

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Aging profoundly impacts the immune system, leading to immunosenescence decline in immune function that increases susceptibility to infections, reduced vaccine efficacy. The cellular and molecular mechanisms of immunological aging, focus on thymic involution, shifts in T-cell subsets, and chronic low-grade inflammation (inflammaging). Research has shown that oxidative stress and mitochondrial dysfunction play a crucial role in accelerating immune aging by damaging cells and impairing their ability to regenerate. One striking example of premature immune aging is seen in rheumatoid arthritis (RA) where T-cells exhibit hallmarks of accelerated aging, including DNA damage accumulation and metabolic dysfunction. Beyond RA, immunosenescence plays a critical role in exacerbating other age-related diseases, emphasizing the need for targeted interventions. Recent research suggests that strategies like caloric restriction, exercise, and immune modulating therapies may help rejuvenate immune function. Furthermore, metabolic reprogramming through interventions aimed at restoring energy balance in aging immune cells offers a promising avenue for mitigating immune decline. Understanding and addressing immunological aging is crucial for extending health span and reducing the burden of age-related diseases.

## **Synergistic Utilization of Cost-Effective Glycerophosphate and Biologically Active Zein for Innovative Minimally Invasive Smart Thermo-Responsive Hydrogels for Potential Hard Tissue Engineering Applications**

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Skeletal defects are the second leading cause of disability worldwide, prompting the development of smart solutions for treatment. Calcium glycerophosphate (Ca-GP), chitosan (CS), hydroxyapatite (HA), and zein (ZN) were used to fabricate these thermo-responsive hydrogels. Ca-GP, an economically viable and bioactive glycerophosphate source, remains relatively underexplored. Natural protein ZN and the gold standard bone regenerative biomaterial HA were incorporated as reinforcing agents. The resulting composite hydrogels (HG) exhibit a sol phase at 4 °C and transition to gels at body temperature within 4 min. Their good injectability and the ability to be easily shaped into complex structures further support their great potential as minimally invasive solutions for treatment. The addition of ZN significantly improved the mechanical and biological properties of the HGs. The highest ZN concentration resulted in the strongest mechanical strength, measuring 52.2 MPa at 40% strain. HGs exhibited optimal swelling and degradation rates. Scanning electron microscopy analysis supported their porous nature. In vitro cell culture, the assays and wound healing assays demonstrated their excellent biocompatibility and regenerative potential. Drug-loaded HGs exhibited up to 90% drug release and antibacterial activity. All these results support their promising potential to support the regeneration of skeletal defects in a minimally invasive manner.

## Main Group Metal-Based Catalysts: A Green Approach for the Synthesis of dihydropyrimidin-2(1H)-thione derivatives

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Catalysis is a fundamental tool in modern synthetic chemistry that plays a significant role in driving efforts toward more sustainable and environmentally friendly chemical processes. Main group metal-based catalysts are drng remarkable attention in process engineering due to their cost-effectiveness, lower toxicity, and higher abundance. The present study highlights the catalytic potential of triphenylgermane, a main group metal-based Lewis acid, in the synthesis of dihydropyrimidin-2(1H)-thione derivatives as an alternate catalytic system to classical Biginelli reaction. The synthesized triphenylgermane catalyst promotes a kinetically favorable reaction mechanism, significantly reducing the reaction time while maintaining high selectivity and yield of the product. A detailed comparative study demonstrates its superior efficiency over existing reported conventional catalysts hence highlighting its potential as a greener and more sustainable alternative catalytic solution. Additionally, the use of such catalysts aligns with the basic principles of green chemistry as they reduce reaction time by diverting the overall reaction mechanism to follow a single kinetic path hence controlling the side reactions that generate unwanted chemical transformations. The present study emphasizes the growing role of main group metal catalysts in advancing sustainable chemical transformations and their promising applications in modern pharmaceutical and material science.

## **Role of Pseudomonas in Air Pollution Control: Microbial Degradation of Pollutants**

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Air pollution from industries, vehicle emissions, and other human activities is growing threat to both the environmental and public health. It contributes to respiratory diseases, climate change and ecosystem damage. Common pollutants include heavy metals, nuclear hydrocarbons, pesticides and as well as greenhouse gases. Microorganisms and plants have strongly been studied, for their importance in biotransformation of such hazardous pollutants into non-toxic chemicals that is ecofriendly. Pseudomonas, which is the most frequently found bacteria in nature, known for adaptability and metabolic capabilities play a crucial role in breaking harmful air pollutants. Thus, microorganisms can degrade volatile organic compound (VOCs), hydrocarbons, and particulate matter using specialized enzymes like monooxygenases and dioxygenases. They are also involved in reducing nitrogen oxides and sulphur oxides which contribute to smog and acid rain. Because of this resilience, Pseudomonas can be effectively used in biofiltration systems, bioreactors and other sustainable air purification technologies. However, Pseudomonas on a large scale, comes with challenges. Maintaining the right conditions-such as temperature, humidity and nutrients-is essential for their activity. Some strains can also pose biosafety risks, requiring careful selection and containment. Additionally Microbial air filtration systems require regular monitoring and can be expensive to maintain. Despite these hurdles, advancements in biotechnology and genetic engineering are helping to improve the effectiveness and cost-efficiency of Pseudomonas-based air pollution control. This is how helpful bacteria like Pseudomonas is helpful in cleaning the environmental pollutants that is harmful for our environment including plants, animals and human beings.



## **Fabrication of Electrospun Nanofibers Using the Extracellular Matrix Derived from Decellularized Umbilical Cord for Tissue Engineering Application**

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Tissue engineering is an optimal solution for tissue regeneration. Therefore, the extracellular matrix (ECM) is used as a natural carrier system, as a source of physical signals and the key modulator of tissue repair and regeneration. Among all the available sources of the scaffold, the human umbilical cord can be regarded as the most suitable one for the scaffold production as this material is a biological waste, and meets the standards that must be provided for the tissue engineering. Therefore, the ECM from the decellularized umbilical cord was used. The prepared decellularized ECM was further reconstituted into nanofibrous scaffolds using electrospinning approach, which provided a nanofibrous structure with interconnected porous network characterized by high porosity, large surface area and efficient interconnectivity, which are fundamental to cell attachment, proliferation and tissue remodeling. The synthesized electrospun fibers were characterized for assessing the physicochemical, mechanical, and biological features. FTIR analysis revealed presence of ECM components within fibers and SEM analysis of fibers gave morphological and homogeneity details. Hydrophilicity of the fibers was evaluated by contact angle measurements; moreover, the fiber dimensions were checked with a Scanning Electron Microscopy (SEM). For the assessment of the mechanical properties of the scaffolds, DMA tests were performed which confirmed their usage for load bearing application. Specific functional characterization tests to assess the swelling, porosity and degradation performance under in vitro conditions were presented for evaluating the repertoire of controlled biodegradability. Furthermore, in vitro drug release studies prove the ability of the scaffold to release the drug in a controlled manner. Cell compatibility was established on fibroblast cells and no cytotoxicity was observed.

## Synthesis, Characterization, and Potential Applications of an Organic-Inorganic Hybrid Nanomaterial

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The organic-inorganic hybrid nanomaterials are exciting materials for their potential applications. Different types of organic compounds are used to coordinate with selected metals under specific reaction conditions to afford hybrid nanomaterials. Carboxylic functionalized organic linker has been derived and characterized by UV/VIS, FTIR, TGA, PXRD analyses, and a respective framework has also been synthesized with transition metals and characterized by FTIR, TGA, PXRD, SEM and EDX analyses. The catalytic activity of both products has been investigated as well. 96% conversion efficiency has been achieved with 66% selectivity. The biological activities have also been investigated. The synthesized products are effective antimicrobial agents against several selected microbes. These hybrid materials exhibited excellent catalytic and biological activities. Results revealed that these types of compounds are very important for future research and development.

## Synthesis of Multi-Metallic Porous Nanocomposite having Catalytic Potential for Green Hydrogen Production

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Porous materials with remarkable structural variety and multifunctional qualities are highly demanded for their potential applications. Multi-metallic MOFs are very attractive for applications in heterogeneous catalysis, gas storage, sensing, and energy conversion because the careful selection of metal nodes allows for fine adjustment of physicochemical features. Compared to monometallic and bimetallic counterparts, multi-metallic porous materials show synergistic effects that improve their catalytic activities, electrical characteristics, and stabilities by combining several distinct metal centers into a single composition. Recent developments in synthesis methods, including as hydrothermal, solvothermal, and post-synthetic modification procedures, have made it easier to create these intricate structures with regulated metal distribution. With the encouraging potentials of porous materials, there are still obstacles to overcome in order to achieve consistent metal dispersion, scalability, and long-term stability in operating settings. In this work, a porous nanocomposite was produced on a metallic substrate using a straightforward synthesis technique. FTIR confirmed the chemical bonding and coordination environment, while TGA determined the good thermal stability and composition of tetrametallic MOF-89. PXRD data peaks of MOF-89 and its powder shows higher crystallinity. SEM and EDS results revealed successful synthesis of the designed material. Specifically, the optimized multilevel, hollow nanostructured bifunctional catalyst is effectively used for green hydrogen production. It showed a very high catalytic efficiency from OER results as revealed from overpotential and Tafel slope. Consequently, a low cell voltage of around 1.62 V vs. RHE was achieved with nanocomposite as an electrode material during electrocatalysis. The current work may provide new insights on the discovery and design of multivariate nanocomposite, a potential material for efficient catalysis in real-world applications.

## Synthesis of Transition Metal Based Bifunctional Catalysts for Catalytic Small Molecules

### Activation

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The need for sustainable energy production and its utilization tremendously increasing nowadays that led to large energy depletion in many natural energy sources. There is a need to develop bifunctional catalysts that not only contributes to the green energy synthesis but also to environmental remediation approach by carbon dioxide fixation. Their effective attribution on a single platform is highly in demand. Metal-organic frameworks give very unique properties as heterogeneous catalysts, where the tuneable pore size and unique structures of open channels can attribute both catalytic small molecules activation. In this regard, transition metal-based MOFs are highly in practice as they offer low overpotential, fast charge transfer, better kinetics, stability in different pH media due to their efficient active sites, better conductivity, redox properties, low budget, stability and also their potential for higher oxidation states under electrochemical process. In line with sustainable energy production, carbon dioxide cycloaddition can lead to the production of many useful chemicals of carbonates, methane, formic acid, etc. The CO<sub>2</sub> cycloaddition with epoxides is termed a sustainable approach due to 100% stoichiometric efficiency and abundant atmospheric CO<sub>2</sub> as an effective and non-hazardous C1 molecular precursor. Thus transition metal-based MOFs as bifunctional materials simultaneously offer renewable energy sources and also carbon management.

## Green Extraction of Essential Oils from *Ocimum basilicum* Using Deep Eutectic Solvent: Optimization via RSM and ANN with Evaluation of Antioxidant, Antimicrobial, and Mosquito-Repellent Activities

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*Ocimum basilicum* (Ob), known as Niazbo, is a well-known culinary herb from the Lamiaceae family. The essential oil in (Ob) has numerous medicinal applications, including antimicrobial and antioxidant properties. Deep eutectic solvents are a paradigm in extracting phytochemicals because they are safe, easy to use, and have minimal side effects. Developing greener and safer phytochemical extraction techniques is crucial to reducing environmental risks. Response surface methodology (RSM) and artificial neural networking (ANN) are advanced optimization techniques for optimizing extraction parameters to determine the best extraction conditions. Hydro-distillation method is used for extraction and citric acid and glucose (1:1) DES as an extractant in this present research, while yield optimization of essential oil is investigated using four independent variables, including % of DES (A), DES/sample ratio (B), temperature in degree Celsius (C), and time in minutes (D). Experimentally, the optimal yield obtained is 39.17 mL at 3.16 % (A), 7.18 (B), 70 °C (C), and 210 min (D). The RSM-predicted yield is 43.83 mL, while the ANN-predicted yield is 41.42 mL. Lower %RSD, PPE, RMSE, %AAD, and high R<sup>2</sup> values obtained from ANN show that ANN has better predictive efficiency than RSM. It is also found that ANN-generated outputs are statistically significantly better for yield prediction ( $p < 0.002$ ) as compared to RSM. It is also found that the extracted oil shows antibacterial activity against *E.coli* bacteria with a zone of 28 mm, and the best result showed at the expense of 200 µL. The antioxidant potential of this extracted oil shows excellent antioxidant (DPPH) activity giving IC<sub>50</sub> of 90.36 against 1000 µL DPPH solution. It was also experimentally determined that the extracted oil is mosquito repellent. This research highlights the potential of citric acid/glucose DES.

## Halogen Doped Carbon Ring as Anode Nanomaterial for Na-ion Secondary Batteries; A DFT Study

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Research on the synthesis and design of materials with high energy density is growing. For this reason, efforts are always being designed to form new and upgraded substances. Here, we suggest a novel and useful approach to upgrade the Na-ion batteries voltage and overall performance. Using DFT calculations, to study electronic and energetic properties of C nanoring ( $C^{16}$ ) to form complex with halogens ( $X^-$ ). The complex of halogen doped  $C^{12}$  nanoring is then adsorbed with alkali metal ion  $AM/AM^+$ . As it has potential application to be used as anode material in alkali-ion batteries. The doping of ( $AM/AM^+$ ) alkali metal ion is examined on C nanoring complex doped with halogens. The interaction energy of Na is higher as compared to  $Na^+$  with carbon nano rings. Pure C nanoring show cell voltage of lower value (-1.34 V for  $C^{16}$ ), and it can be significantly increased when it is doped with halogens. Doping of halides increases the Gibbs free energy which in turn results in higher cell voltage. It is clear from the results that electronegativity is directly proportional to cell voltage. Cell voltage obtained ranges from 1.87 to 1.86 V. It is clear from calculations that  $C^{16}$  gives the most accurate and suitable cell voltage of 1.86, 1.87 and 2.01 V in case of  $Br^- @C^{16}$ ,  $Cl^- @C^{16}$  and  $F^- @C^{16}$  respectively. From results, it is obvious that by doping pure C nanoring with halogens proves potential material as anode for Na- ion secondary battery as a potential replacement to existing ones.

## Synthesis and Characterization of Bismuth Based Nanocomposites and Their Application

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Using a sequence of chemical reactions and hydrothermal techniques, we produced  $\text{Fe}_3\text{O}_4$  and  $\text{BiVO}_4$  nanoparticles. Then,  $\text{Fe}_3\text{O}_4$  was added to the  $\text{BiVO}_4$  to create a hybrid  $\text{Fe}_3\text{O}_4/\text{BiVO}_4$  nanocomposite. Additionally,  $\text{Fe}_3\text{O}_4/\text{BiVO}_4$  composites were doped using different  $\text{AgCl}$  concentrations. A different number of solutions have been prepared with (5%, 10%, 15% and 20%) of Chloride composites. The morphology of these generated nanocomposites was assessed using FTIR and SEM techniques. It has been confirmed that sample is having high surface area, uniformity and porosity. The components that are produced can be applied to environmental remediation. Methylene blue degradation in the presence of sunlight was used to evaluate the photocatalytic performance of composites, and UV-visible spectroscopy verified both their successful synthesis and photocatalytic qualities.

## **Bacteriophage Therapy: A Game Changer in the Fight Against Antibiotic-Resistant Superbugs mainly Klebsiella Pneumoniae**

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The emergence of antibiotic-resistant "superbugs" like *Klebsiella pneumoniae* and other resistant bacterial strains, is a lethal complicating agent in international public health, deserving of alternative treatment approaches. According to a 2019 WHO report, drug-resistant bacteria caused about 1.27 million deaths, mainly due to infections like drug-resistant *Klebsiella pneumoniae*. By 2050, the deaths can surpass cancer deaths. In response, phage therapy has been viewed as a substitute for antibiotics. Bacteria that are resistant are multiplying more quickly than antibiotics can be invented. This is recalling us to a period prior to antibiotics. According to the recent research *Klebsiella pneumoniae*, a resilient bacterium of the Enterobacteriaceae genus, is particularly challenging since it produces a capsule that shields it from the immune system as well as from antibiotics. Bacteriophage therapy using viruses that selectively infect and kill bacteria has emerged as such a promising means due to its high specificity.

Genetic engineering developments, phage combinations, and targeted phage therapy have greatly promoted its clinical significance. In this review, we address new advances in bacteriophage therapy, its mechanism of action, and effectiveness against multidrug-resistant *Klebsiella pneumoniae*. Regulatory issues, safety, and complementarity between phage therapy and traditional antibiotics are also discussed.

Although recent trials of clinical intervention have demonstrated cure effectiveness against recalcitrant infections, there remains a need to fine-tune treatment regimes in order to offset limitations. Finally, bacteriophage treatment represents a revolutionary approach to tackling antibiotic resistance and offers hope for a future when superbugs like *Klebsiella pneumoniae* are no longer an unbeatable menace.



## POSTER PRESENTATION

### Synthesis of Te@CoS/S-g-C<sub>3</sub>N<sub>4</sub> for Efficient Removal of Organic Pollutants under Sunlight Irradiation

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Industrial effluents from industries are causing notable water pollution. The polluted water bodies affect broader diversity in aquatic ecosystems. It is crucial to manage outfall pollutants such as dyes, fertilizers, and pharmaceuticals in order to tackle this hazard. In this consideration, different photocatalysts that degrade waste materials from the petrochemical industries have been effectively responsible for the environmental degradation of a number of organic pollutants. The CoS NPs, Te@CoS NPs, and Te@CoS/SGCN NCs catalysts were synthesized using co-precipitation techniques before they could be employed in the degradation of methylene blue (MB), an organic dye. The photocatalytic results were shown as; cobalt sulfide degrading the MB upto 70%, tellurium doped NPs gave the degradation results upto 86%, and SGCN doped composites extended this degradation upto 97%. The increase in % degradation is due to the electron recombination in the conduction and valence bands. The modification of cobalt sulfide with tellurium and SGCN structure proved to be a fruitful approach which resulted in excellent performance.

**Keywords:** Photocatalysis, FTIR, Semiconductor photocatalysts, sulfides, Sustainable pollution treatment, Environmental remediation.

## **ZnO-Embedded Polyelectrolyte Multilayers for Nanofiltration Membranes to Combat Fouling and Bacterial Colonization in Water Filtration**

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The study demonstrates the preparation of ZnO-embedded polyelectrolyte multilayers (PEMs) based NF membranes for water treatment. The process of membrane separation is the most efficient but suffers with fouling problems, for this reason polyelectrolyte multilayers based thin film composite (TFC), asymmetric membranes were prepared by embedding Zinc oxide nanoparticles (ZnO-Np). Polyether sulfone (PES) polymer is used to prepare the ultrafiltration (UF) support via non-induced phase inversion process (NIPS) on a non-woven polypropylene support. To prepare nanofiltration membranes, UF support is then coated with PEMs of polyelectrolytes (PAH/PSS) in a layer-by-layer assembly fashion, which were then crosslinked by glutaraldehyde (GA). In the final layer of PEMs ZnO-Np are embedded via dip coating followed by crosslinking. Performance evaluation of the membranes is carried out in terms of water permeability, dye rejection and fouling tests with common foulant (i.e., Bovine serum albumin, and E. coli). The results show that embedding ZnO nano particles in membrane significantly enhanced the hydrophilicity of prepared NF membranes. The fouling tests indicate significant resistance against the foulant and complete killing of the bacteria on the ZnO-embedded PEM based membranes compared to PES and PEM based membrane without ZnO. The characterization of the ZnO nanoparticles was done through FTIR, SEM, XRD, and zeta sizer and membranes were done through FTIR, SEM, AFM and contact angle measurements.

## Designing Highly Potential Photocatalyst Comprising Zn@CoFe<sub>2</sub>O<sub>4</sub> with S@G-C<sub>3</sub>N<sub>4</sub> Ternary Composite

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Water contamination is majorly caused by industrial effluents, which result in significant harm to aquatic ecosystems and environmental sustainability. Such effluents include dyes, fertilizers, and pharmaceutical residues, which call for prior treatment before being released from industries to overcome their adverse effects. Among other techniques, photocatalysis has been attractive because it provides an efficient environmental-friendly alternative for degrading organic pollutants under solar irradiation. The present study deals with the co-precipitation method of synthesizing an advanced photocatalyst for degradation of methylene blue (MB) dye. It also investigated various synthesis methods applicable to nanoparticles and nanocomposites, in addition to employing appropriate structural and optical characterization techniques. Synthesis of Zn@CoFe<sub>2</sub>O<sub>4</sub> nanoparticles was achieved through co-precipitation, while sulfur-doped graphitic carbon nitride was prepared by calcining thiourea to obtain the Zn@CoFe<sub>2</sub>O<sub>4</sub>/S@G-C<sub>3</sub>N<sub>4</sub> NCs and utilized in photocatalysis evaluation. The synthesized photocatalyst was characterized using Fourier-transform infrared spectroscopy (FTIR) and UV-Vis spectroscopy for structural and optical properties. Photocatalytic activity measurements further indicated that 30% S@G-C<sub>3</sub>N<sub>4</sub>/8% Zn@CoFe<sub>2</sub>O<sub>4</sub> NCs had the best MB degradation under sunlight. The enhanced degradation efficiencies are attributed to the synergetic interaction between Zn@CoFe<sub>2</sub>O<sub>4</sub> and S@G-C<sub>3</sub>N<sub>4</sub>, which leads to efficient charge separation and minimization of electron-hole recombination. This illustrates great applicability in the sewage treatment of engineered nanocomposites and underlines the importance of material modification to improve photocatalytic performance.

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**Synthesis of Mn-CoS Nanoparticles for Efficient Removal of Organic Pollutants.**

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The world is facing a huge crisis in the form of water pollution. Water contamination is not only affecting the intricate balance of the aquatic ecosystem but also poses a threat to human health, climate and water availability. Organic dyes are one of the major water pollutants which can be degraded to improve the quality of water and prevent water pollution for which photocatalysis is an eco-friendly option. This study aims to synthesize an efficient metal sulfide photocatalyst that effectively degrades organic dyes under sunlight. For this purpose, CoS, 1% Mn-CoS and 5% Mn-CoS nanoparticles were synthesized using the coprecipitation method, which is simple, quick and relatively inexpensive. Methylene blue was used as the standard dye. Its photocatalytic degradation was determined using the UV-Vis spectrophotometer by analyzing the concentration of methylene blue at intervals of 20 minutes. It was observed that 5% Mn-CoS showed the best degradation rate among the three nano catalysts synthesized. This study signifies the use of photocatalysts for wastewater treatment and how Mn doping can enhance the photocatalytic performance of CoS. Dye degradation using photocatalysis aligns with sustainable development goal 6 by improving water quality and reducing water pollution.

## Alginate Grafted Acrylic Ter Polymer Nanocomposites for Adsorption of Pollutants from Waste Water

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Wastewater treatment has benefited from the substantial rise in popularity of alginate-grafted acrylic terpolymer nanocomposites as adsorbents. Hybrid materials which unite alginate biocompatible properties with acrylic polymer mechanical robustness and chemical resistance operations as effective adsorbents in wastewater treatment. The hybrid materials prove highly efficient in pollutant removal operations. The production of these nanocomposites requires free radical polymerization procedures which add various times. The use of TiO<sub>2</sub>, nanoparticles increase the adsorption capacity of these materials. The success of the grafting process is confirmed through characterization using methods which include FTIR, SEM, TGA and XRD. Nanocomposite adsorption performance depends on several parameters including pH value together with adsorbent concentration and temperature while following pseudo-second-order kinetics models and Freundlich isotherm patterns. The adsorption process follows pseudo-second-order kinetics together with Freundlich isotherm models. Strong electrostatic interactions and hydrogen bonds and  $\pi$ - $\pi$  interactions exist between these nanocomposites. The pollutant removal capability of the nanocomposites boosts because of hydrogen bonding and electrostatic forces alongside  $\pi$ - $\pi$  interactions. Experts show that efficient regeneration procedures enable these materials to keep their adsorption ability after repeated usage. The combination of superior adsorption performance together with ease of reuse makes alginate-grafted acrylic nanocomposites function as a viable wastewater treatment solution. The research should move forward by improving synthesis conditions and testing the applicability with different types of pollutants.

**Keywords.** Calcium alginate, nanocomposites, polymers, wastewater treatment, regeneration, biodegradable, pollutant removal

## Computer-aided Analysis of Phytochemicals as Potential SARS-COV 2 Inhibitors Based on Molecular Docking, ADMET and DFT Studies.

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Coronaviruses are known to cause diseases related to the respiratory tract. They were first discovered in the 1960s and were thought to be relatively harmless until the breakout of SARS-COV in 2002 and MERS in 2012. In 2019 SARS-COV-2 broke out and resulted in millions of people being affected and declared a global pandemic in January 2020, mutating into several variants such as Alpha, Beta, Gamma, Delta, and omicron. Several vaccines are available but are plagued with dwindling low immunity issues and no long-term protection. In this study, we have targeted the RBD of the SARS-COV-2 Omicron variant. The pharmacokinetics and pharmacological characteristics of nearly two hundred substances were evaluated, and twenty-nine were screened for pharmacokinetics and pharmacological characteristics. Which further were docked against the target protein. The binding affinity was calculated via molecular docking, the reactivity of compounds was evaluated using DFT, and the stability was analyzed using MD simulations. It was concluded that phytochemicals such as Withanolide E, Kaempferol, and Ledebouriellol might be potential inhibitors for targeted protein after extensive in vitro and in vivo testing.

## ***Curcuma zedoaria* Mediated Bio-Fabrication of MnO:ZnO Nanocomposites and Their Biological Potential and Semiconducting Properties**

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Metal-based nanoparticles offer immense potential as pharmacological agents apart from possessing interesting electrical properties. To harness these potentials, manganese oxide:zinc oxide nanoparticles were fabricated using crude extract of *Curcuma zedoaria*. The fabricated nanoparticles were found to be thermally stable and crystalline. Synthesized with different metal ratios, the nanocomposites exhibited significant anti-microbial and DPPH radical scavenging activities. Moreover, strong anti-leishmanial activity was shown by all the composites with IC<sub>50</sub> values of 0.03, 0.14, and 4.3 µg/mL. The nanocomposites also displayed optimum energy storage and semiconducting abilities. The band gaps were found to be between 3.26 and 3.11 eV. Optimum values of dielectric constant (~ 0.95) and capacitance (~1.0 pF) were observed for MnO<sub>2</sub>:ZnO, while the MnO<sub>1</sub>:ZnO<sub>2</sub> composite exhibited the best AC conductivity (1.8 Å—10<sup>-9</sup> S/m). These studies depict the potential of these nanocomposites as pharmacological agents, as well as possessing tendency to be used as semiconducting devices.

**Keywords:** Bimetallic nanocomposite, *Curcuma zedoaria*, Anti-leishmanial activity, Anti-microbial activity, Antioxidant, Semiconductor.

## Synthesis, Characterization and Practical Applications of Ethylene Vinyl Acetate (EVA) Copolymer-Based Composites with Enhanced UV-Resistant Properties

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The composites based on ethylene vinyl acetate (EVA) copolymer are becoming increasingly popular for their exceptional properties, especially the incorporation of different additives that make them UV resistant. Several materials have been used to enhance the UV resistance of EVA composites, like fuller's earth clay, 2-ethylhexyl acrylate (2-EHA), carbon nanoparticles (CNPs), aluminum silicate, graphite powder, titanium dioxide (TiO<sub>2</sub>), and cerium oxide (CeO). Fuller's earth clay, a naturally occurring magnesium aluminum silicate clay that is used for skin and hair care products because of its absorbent ability, works in conjunction with EVA composites as a filler which improves their mechanical properties along with its UV resistance. The compatibilizing effect aiding the interfacial bonding between EVA and inorganic fillers is contributed by the added 2-EHA. Because of their high surface area to volume ratio at nanoscale, CNPs enhance the UV shielding property of the composites. The addition of graphite powder increases the electrical conductivity and provides additional UV shielding. The rest of the materials, TiO<sub>2</sub>, ZnO, MgO, and CeO, serve the purpose of active UV blockers, absorbing harmful rays and prevent degradation of polymers. The structural, morphologic, and optical features were analyzed by using techniques such as Thermogravimetric Analysis (TGA), Fourier-transform infrared spectroscopy (FTIR), Differential Scanning Calorimetry (DSC), scanning electron microscopy (SEM), UV-visible (UV-vis) spectroscopy, X-ray diffraction (XRD). The combination of these additives enables the fabrication EVA composites with increased mechanical properties, greater thermal stability, and superior resistance to UV radiation, making them useful for automotive parts, packaging products, and outdoor goods exposed to UV radiation.

**Key words:** Ethylene vinyl acetate copolymer (EVA), UV-resistant properties, fuller's earth clay.



## Comparative Analysis of Potential of *Aloe vera* as Anti-Cancer Agent

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*Aloe vera*, a plant with a rich history in traditional medicine, is now being investigated for its potential anticancer properties. However, its diverse chemical composition also raises concerns about toxicity and safety. This research on *Aloe vera*, focusing on its key components, anticancer activity, and associated risks. *Aloe vera* comprises a complex mixture of compounds, including vitamins, sterols, polysaccharides, and anthraquinones like aloin and emodin. Studies have explored its efficacy against various cancers, with some success in inducing apoptosis and inhibiting cancer cell growth. Novel drug delivery systems like phytosomes are being developed to enhance bioavailability and reduce side effects. However, potential toxicities, including hepatic damage and mutagenic effects from anthraquinones, necessitate careful evaluation. Recent safety evaluations suggest *Aloe vera* barbadensis extract C (AVBEC) does not cause organ toxicity or immune system damage in rats. HPLC-MS/MS analysis has identified key components in AVBEC, such as malic acid, which, while abundant, can induce cell necrosis. *Aloe vera* shows promise as a potential anticancer agent, but further controlled studies are needed to fully elucidate its mechanisms of action, optimize delivery methods, and comprehensively assess its safety profile. Future research should focus on isolating and testing specific components to maximize therapeutic benefits while minimizing risks.

**Key words:** *Aloe vera*, aloin, emodin, apoptosis, phytosomes, cytotoxicity.

## Comparative Phytochemical Analysis and Therapeutic potential of Annona Species in Nutraceutical and Oncology Research

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*Annona crassiflora* known as marolo fruit is an indigenous plant of central Brazil. *Annona Cherimola* known as cherimoya and *Annona atemoya* found Taiwan which are used as teas because of low toxicity whereas Soursop known as *Annona Muricata* Linn used as medicine due to anti-inflammatory and anti-cancer properties. The biological properties and antioxidant activities together with the phytochemical profiles of *Annona* species mentioned above have been examined. These examinations were performed to assess the chemical composition, antioxidant capabilities and their great health benefits. Antioxidant and antiproliferative effects revealed in the phytochemical analyses of these species due to presence of phenolic compounds, flavonoids among alkaloids in them. Especially, *Annona muricata* showed antioxidant activity with an IC<sub>50</sub> value of 141.127 µg/mL with bioactive compounds i.e., flavonoids, phenolics, steroids, alkaloids and saponins. In comparison both of the *Annona cherimola* and *Annona atemoya* showed phenolic content especially proanthocyanidins which resulted in the antiproliferative effects against HeLa and HepG2 cancer cell lines, exhibiting chemoprevention. *Annona crassiflora* displayed strong antioxidant activity with an EI<sub>50</sub> of 182.54 µg/mL and exhibited a great amount of cytotoxicity against U251 glioma cells (GI<sub>50</sub> = 21.34 µg/Ml), comparable to the effects of doxorubicin. All the findings underscore the nutraceutical potential of *Annona* species because of notable anticancer and antioxidant properties. While *Annona muricata* is accepted as an antioxidant agent, *Annona cherimola* along with *Annona atemoya* are accepted as dietary supplements that are used to influence redox balance and chemo-preventive benefits. These researches gave understandings for the advancements on health products that force the diverse bioactive properties inherent in the *Annona* species.

## Synthesis of Biogenic Silver Nano propolis for Burn Wound Treatment

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Burn wound healing remains a critical challenge, and there is an increasing need for effective and cost-efficient treatments. This study explores the synthesis of Silver nanopropolis via a green approach, for burn wound healing treatment. Bee propolis, sourced from northeast Punjab, Pakistan, was extracted using maceration and analyzed for its high phenolic content, and utilized to reduce silver ions to prepare nanoparticles. The synthesized nanopropolis was characterized by using UV-Visible Spectroscopy (UV-Vis), Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), and X-ray Diffraction (XRD). Nanopropolis showed significant antioxidant ( $0.4696 \text{ } \mu\text{g}$ ) and anti-inflammatory ( $0.3996 \text{ } \mu\text{g}$ ), and antibacterial activity. An ointment formulated with silver nanopropolis and hydrogels was studied to treat burn wounds in rabbits. The results showed faster wound healing and more collagen deposition silver nanopropolis treated wounds compared to the control group.

## Zinc Oxide Nanoparticles Based Efficient Electrochemical Sensors For The Simultaneous Detection Of Metal Ions

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Rapid industrialization in Lahore, Pakistan, has led to significant groundwater contamination by heavy metals, posing severe public health risks. This study developed a cost-effective method for detecting lead ( $Pb^{2+}$ ), cadmium ( $Cd^{2+}$ ), and chromium ( $Cr^{3+}/Cr^{6+}$ ) in wastewater. Zinc oxide nanoparticles (ZnO-NPs) were synthesized via a sol-gel method using zinc acetate dihydrate, resulting in flower-like nanoparticles with an average size of 20 nm. These ZnO-NPs were incorporated into a polyvinylidene fluoride (PVDF) composite film and drop-cast onto carbon cloth to fabricate a modified electrode. The ZnO nanoparticles were characterized using UV-Visible and Fourier Transform Infrared (FTIR) spectroscopy, Scanning Electron Microscopy (SEM), and X-ray Diffraction (XRD). The modified electrode's performance was evaluated through cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and differential pulse voltammetry (DPV) for the detection of heavy metal ions  $Pb^{2+}$ ,  $Cd^{2+}$ , and  $Cr^{3+}/Cr^{6+}$  in wastewater. The electrode exhibited rapid, sensitive, and reliable detection, meeting international water quality standards. This highlights the potential of ZnO-NPs-based electrodes as an efficient and cost-effective solution for addressing heavy metal contamination in industrial wastewater. The study emphasizes the role of innovative sensing technologies in reducing health risks, protecting the environment, and advancing Sustainable Development Goal (SDG) 3 by raising awareness about the dangers of contaminated wastewater to vulnerable communities near industrial zones.

# Unlocking Nanoparticle Potential: A Machine Learning Approach to Predict and Optimize Band Gaps of ZnS

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Accurate band gap prediction in nanoparticles is crucial for applications spanning catalysis, solar energy, and environmental remediation. This study investigates machine learning (ML) for predicting zinc sulfide (ZnS) nanoparticle band gaps, a widely studied and technologically relevant material. Band gap data from UV-Vis spectrophotometry and literature were used to train and validate five ML models: Support Vector Machine Regression (SVR), Instance-Based k-Nearest Neighbors (IBK-KNN), Random Tree (RT), Multilayer Perceptron (MLP), and Additive Regression (AD). The models demonstrated significant performance, enabling enhanced understanding and optimization of ZnS band gap behavior. This ML approach provides a rapid, cost-effective alternative to experimental characterization, accelerating the design and application of ZnS nanomaterials in diverse technological fields. The developed models facilitate efficient nanomaterial optimization and discovery, ultimately contributing to advanced material design.

## Robust Synthesis of New Spiropyrazoline in Deep Eutectic Solvent

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Spiropyrazolines are the compound having a unique spirocyclic junction where two rings converge at the C-5 Carbon. These spirocyclic molecules are significant interest to both medicinal and synthetic chemists due their enriched bio-profile. Conventional methods often employ volatile organic solvents which poses significant threat to environment. In this research, deep eutectic solvents have been used and compared with ethanol for the synthesis of spiropyrazolines, providing a more sustainable and environment friendly synthetic approach. All derivatives were confirmed by spectroscopic techniques. This method utilized mild reaction conditions which resulted in improved yield, reduced reaction time and minimal complexities.

## Silica-Acid Catalyzed Synthesis of O-Alkyl Glycosides: A Green Approach for Drug Delivery

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The biological profile of Alkyl glycosides makes them a potential candidate for drug delivery system. In this study, a biodegradable drug carrier system was developed through the chemical modification of naturally occurring monosaccharides with aliphatic alcohols, leading to the formation of alkyl O-glycosides. The structure confirmation was achieved by Fourier-transform infrared spectroscopy (FTIR), nuclear magnetic resonance ( $^1\text{H}$  NMR), and X-ray diffraction (XRD) techniques. The thermotropic and lyotropic behavior of these glycosides was evaluated via differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and optical microscopy. The drug delivery potential of the formulations was assessed in vitro using aspirin as a model drug, with release profiles monitored by UV-visible spectrophotometry. The results demonstrated effective and sustained drug release of the entrapped drug, indicating that alkyl O-glycosides are potential and cost-effective drug delivery systems with enhanced therapeutic efficacy. This work aligns with SDG 3: Good Health and Well-Being, by improving therapeutic outcomes, enabling sustained drug release, and minimizing side effects.

## Microwave Assisted Synthesis of Anti Inflammatory Oxazoles

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Inflammatory disorders cause to severe health complications, often leading to chronic diseases that significantly reduces the quality of life. This study focuses on the green synthesis of anti-inflammatory oxazole derivatives employing microwave radiations via a Schiff base of coumarin. The hetroannulation achieved with acetyl coumarin catalyzed by iodine under the influence of microwaves. The synthesized oxazole derivatives were characterized using spectroscopic techniques, including FTIR,  $^1\text{H}$ NMR, and EIMS. Their pharmacological potential was assessed, revealing notable antioxidant by DPPH assay and anti-inflammatory studies by HRBC membrane stabilization method. These findings highlighted the efficient and practical approach adopted for synthesis of targeted bioactive oxazoles that can be utilized to reduce the inflammation.



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## Chitosan Hydrogels for Sustained Vitamin D3 Release

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The low bioavailability and potential loss of bioactivity during oral delivery exacerbate Vitamin D3 deficiency which emphasizes the need for the development of a sustained release system. In this study cost-effective, and eco-friendly polymeric blends of chitosan and sago starch as sustainable nutraceutical carriers (CS 1-4) of Vitamin D3 has been synthesized. All prepared hydrogels were confirmed by FTIR, XRD and SEM analysis. The swelling studies reveal the pH-responsive behaviour of these blends, affirming their potential for sustainable release. Furthermore, it's release predominantly follows zero-order kinetics, indicating a controlled release mechanism significantly influenced by the concentration of chitosan. These prepared samples were biocompatible and biodegradable and provide sustainable material for good health and wellbeing.

**Keywords:** Vitamin D3, Chitosan, nutraceutical carrier, in vitro sustained release, SDG-3

## Neem-Derived Graphene Quantum Dots for Sustainable Nanotechnology

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Graphene Quantum Dots (GQDs) are valuable in bioimaging and drug delivery due to their unique properties. Traditional synthesis methods often employ toxic chemicals and non-renewable resources creating environmental hazards. This research utilizes a simple, environment friendly method to synthesize GQDs from neem tree leaves using a water-based heating process at 200°C, seeking a cleaner, more sustainable approach. Readily available neem leaves were hydrothermally treated to afford GQDs, and doped with Boron to enhance their properties. The prepared GQDs were confirmed by UV and FTIR spectroscopic techniques. The abundant, renewable precursor avoids toxic chemicals, making it a "green" alternative to traditional methods and demonstrates utilization of natural sources for nanomaterial synthesis. This method offers a sustainable route for GQD preparation. This research approach promotes a benign method and highlights the potential of plant-based materials for future innovations.

## Sustainable Leather Production: Eco-Friendly Alternatives to Chrome Tanning

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The tannery industry is a well-established and heavily industrialized sector that plays a crucial role in the global economy. However, the conventional chrome tanning method poses significant environmental and health risks due to the oxidation and release of toxic, carcinogenic hexavalent chromium ( $\text{Cr}^{6+}$ ). This has driven the development of alternative tanning systems aimed at reducing these hazards. One approach involves using chrome-free tanning agents, such as synthetic tanning salts and polymeric agents, to eliminate chromium discharge. Another strategy enhances the exhaustion rate of chrome tanning through nanomaterials like methyl methacrylate and n-butyl acrylate. Additionally, chrome recovery and reuse plants can extract chromium from tannery effluents for sustainable recycling. Emerging alternatives with promising eco-friendly potential include the Tara tannin-Zeolite (TA-ZE) system, biomass-derived tanning agents such as Î²-TCD and Î²-GCD, vegetable tannins, and a triazine-based syntan with active chlorine groups (SACC). These innovations offer leather with desirable properties while minimizing hazardous substances like  $\text{Cr(VI)}$ , contributing to a more sustainable leather manufacturing process.

## Probing the Binding Mechanism and Kinetics of Amphiphilic Acrylate Copolymers with Bovine Serum Albumin

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This article presents that acrylate copolymers are the potential candidate against the adsorption of bovine serum albumin (BSA). A series of copolymers poly(methyl methacrylate) (pMMA), poly(3-sulfopropyl methacrylate-co-methyl methacrylate) p(SPMA-co-MMA), and poly(dimethylaminoethyl methacrylate-co-methyl methacrylate) p(DMAEMA-co-MMA) were synthesized via free radical polymerization. These amphiphilic copolymers are thermally stable with a glass transition temperature ( $T_g$ ) 50–120 °C and observed the impact of surface charge on amphiphilic copolymers to control interactions with the bovine serum albumin (BSA). These copolymers pMD1 and pMS1 have surface charges, - 56.6 and - 72.6 mV at pH 7.4 in PBS buffer solution that controls the adsorption capacity of bovine serum albumin (BSA) on polymers surface. Atomic force microscopy (AFM) analysis showed minimum roughness of 0.324 nm and 0.474 nm for pMS1 and pMD1. Kinetic studies for BSA adsorption on these amphiphilic copolymers showed the best fitting of the pseudo-first-order model that showed physisorption and attained at 25 °C and pH 7.4 within 24 h.

**Key Words:** copolymer, amphiphilic, bovine serum albumin, kinetic studies, physisorption.

## Composite Material having Bismuth Molybdate, Tungstate And Vanadate With Fe<sub>3</sub>O<sub>4</sub> and Ag<sub>2</sub>S

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This study investigates the synthesis and characterization of a composite material integrating bismuth molybdate, tungstate, and vanadate with Fe<sub>3</sub>O<sub>4</sub> and Ag<sub>2</sub>S. The composite aims to leverage the synergistic properties of these components for enhanced photocatalytic and magnetic applications. Fe<sub>3</sub>O<sub>4</sub> nanoparticles provide magnetic separability, while Ag<sub>2</sub>S enhances the material's visible light absorption and conductivity. The bismuth-based compounds contribute to the material's photocatalytic activity. The composite was synthesized using a co-precipitation method. Characterization techniques, including XRD, TEM, and XPS, were employed to analyze the structural, morphological, and chemical properties. Preliminary results demonstrate to improved photocatalytic degradation of a model pollutant or enhanced magnetic response. This composite holds potential for applications in environmental remediation and magnetic separation.

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## Synthesis of Mn-CoS Nanoparticles for Efficient Removal of Organic Pollutants

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The world is facing a huge crisis in the form of water pollution. Water contamination is not only affecting the intricate balance of the aquatic ecosystem but also poses a threat to human health, climate and water availability. Organic dyes are one of the major water pollutants which can be degraded to improve the quality of water and prevent water pollution for which photocatalysis is an eco-friendly option. This study aims to synthesize an efficient metal sulfide photocatalyst that effectively degrades organic dyes under sunlight. For this purpose, CoS, 1% Mn-CoS and 5% Mn-CoS nanoparticles were synthesized using the coprecipitation method, which is simple, quick and relatively inexpensive. Methylene blue was used as the standard dye. Its photocatalytic degradation was determined using the UV-Vis spectrophotometer by analyzing the concentration of methylene blue at intervals of 20 minutes. It was observed that 5% Mn-CoS showed the best degradation rate among the three nano catalysts synthesized. This study signifies the use of photocatalysts for wastewater treatment and how Mn doping can enhance the photocatalytic performance of CoS. Dye degradation using photocatalysis aligns with sustainable development goal 6 by improving water quality and reducing water pollution.

## **Shampoo Bar and How it Replaces Traditional Shampoo Bottles and Reduce Pollution**

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This study presents the formulation of an advanced organic shampoo bar designed to deliver effective cleansing, deep nourishment, and scalp health while adhering to sustainable and eco-friendly principles. The formulation incorporates mild, sulphate-free surfactants Soapnut powder, Sodium Lauryl Sulfoacetate (SLSA), and Cocamidopropyl Betaine to ensure a rich, gentle lather that cleanses without stripping natural oils. A carefully selected blend of botanical oils (Coconut, Olive, Jojoba, and Argan) enhances hydration, while conditioning agents such as BTMS-50, Hydrolysed Keratin, and Panthenol restore strength, smoothness, and manageability. Structural integrity and longevity are enhanced with Cetearyl Alcohol and Stearic Acid, ensuring durability and extended use. The formulation is pH-balanced (4.5-5.5) to maintain hair health, and GeoGard 221 is included as a natural preservative for broad-spectrum microbial protection. This shampoo bar offers a high-performance, zero-waste alternative to conventional liquid shampoos, aligning with modern consumer preferences for sustainable, salon-quality hair care solutions

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## **Economical Synthesis of Biodiesel by using Chicken Bone Derived Copper Doped Calcium Oxide and Cobalt Doped Calcium Oxide Catalysts**

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The aim of the study was to investigate the feasibility of CaO-doped heterogeneous catalysts for synthesizing biodiesel from waste cooking oil via the transesterification method. The key catalyst, CaO, was extracted from waste chicken bones through calcination at 900°C. Later, the same catalyst was used as a substrate for doping with copper and cobalt to prepare Cu-doped CaO and Co-doped catalysts. Similar to the catalysts, the primary feedstock for biodiesel production was waste cooking oil, highlighting that the environment was preferably considered in this study at every stage. The characterization of the catalysts was done by SEM-EDX and FTIR. Later, the workability of the catalysts was tested through several attempts by varying factors such as catalyst amount, reaction time, temperature, and oil/methanol ratio. The prepared biodiesel was analyzed using GC-MS, followed by testing its properties such as viscosity, cloud point, flash point, and density. Results confirmed the feasibility of the doped catalysts for biodiesel production, affirming that the study contributes to recycling biomass for sustainable fuel generation.



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## **The Chemistry Behind Happiness**

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Happiness has its roots in the biochemical changes that take place in the human brain. Mood-altering neurotransmitters like dopamine, serotonin, oxytocin, and endorphins regulate mood, pleasure, and emotional health. These chemicals interact with neural pathways, influenced by external factors like socialization, exercise, and diet. Knowing more about the chemistry of happiness can help create interventions to improve well-being, or manage mental health conditions and optimize lifestyle choices. In this paper, we will discuss the biochemical basis of happiness, factors that influence neurotransmitter levels, and ways to naturally boost mood through scientific and lifestyle interventions.

## **Investigating Pakistani Public Perceptions & Attitudes Regarding Lab Grown Meat**

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According to the Food and Agriculture Organization (FAO), the global population of 8.2 billion is expected to be 9.7 billion by 2050 and 10.3 billion by 2080. As the global population increases rapidly, 70% more food is needed to fulfill the global requirement which is troublesome due to limited resources and arable land. On the other hand, Pakistan, with a rapidly growing population exceeding 240 million, faces severe food security and water scarcity challenges, ranking among the most water-stressed countries in the world. The country's dependence on conventional meat production further exacerbates resource depletion, making sustainable food alternatives increasingly necessary. Lab-grown meat, the alternative to conventional meat, is an emerging biotechnology that offers a promising solution by tackling the impediments of an increasing population. Lab-grown meat lowers greenhouse gas emissions by up to 96% as conventional meat production particularly livestock farming is estimated to account for approximately 14.5% of these emissions and uses approximately 89% less water and 99% less land. Furthermore, cultivated meat also mitigates ethical concerns encompassing animal welfare, health concerns arising from the overuse of antibiotics and animal-borne diseases. This study explores public perceptions of lab-grown meat in Pakistan, assessing awareness, willingness to try, and key concerns and influencing factors. A quantitative survey was conducted, targeting diverse demographic groups, and data analysis was performed using descriptive and inferential statistics. The results indicate low familiarity with lab-grown meat, with 46% of respondents unaware of its existence. Females exhibited greater awareness and willingness to try it, although they expressed higher safety concerns compared to males. The study also highlights the need for educational initiatives to enhance consumer acceptance. Public awareness campaigns emphasizing safety, sustainability, and ethical benefits could play a crucial role in shaping perceptions. Addressing pricing, religious acceptability, and regulatory challenges will be essential for the successful integration of lab-grown meat into Pakistan's food system.

## Robust Synthesis of New Spiropyrazoline in Deep Eutectic Solvent

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Spiropyrazolines are the compound having a unique spirocyclic junction where two rings converge at the C-5 Carbon. These spirocyclic molecules are significant interest to both medicinal and synthetic chemists due their enriched bio-profile. Conventional methods often employ volatile organic solvents which poses significant threat to environment. In this research, deep eutectic solvents have been used and compared with ethanol for the synthesis of spiropyrazolines, providing a more sustainable and environment friendly synthetic approach. All derivatives were confirmed by spectroscopic techniques. This method utilized mild reaction conditions which resulted in improved yield, reduced reaction time and minimal complexities.

## **Preparation and Characterization of *A. Barbadensis* (Alovera Gel) and *Punica Granatum* (Pomegranate Juice) Based Anti-Aging Cream for Skin Care**

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The natural process of aging causes the structure of the skin to deteriorate, leading to wrinkles, decreased suppleness, and decreased moisture. The market for anti-aging treatments has grown as people look for formulas that are both natural and effective. By analyzing its main components, this study investigates the composition and effectiveness of an anti-aging cream with pomegranate extract. Antioxidants, especially punicalagins and ellagic acid, which fight oxidative stress and encourage collagen production, are abundant in pomegranates (*Punica granatum*). Additional components that support hydration, skin barrier restoration, and anti-inflammatory properties include glycerin, jojoba oil, aloe vera, and essential oils. The DPPH assay was used to measure the antioxidant potential and ascertain the scavenging activity of free radicals. The components' synergistic functions in skin regeneration are shown by a comparative investigation. According to the findings, pomegranate-based skincare products show promise since they may offer significant anti-aging advantages.

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## Functionalized PVA Composites for Wastewater Remediation

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Heavy metals in water resources causes serious health hazards due to their toxicity and persistence. This study explores the potential of polyvinyl alcohol (PVA) composites blended with coconut ash and guar gum. The coconut husk ash was activated by acid to enhance its surface area, porosity, and active sites, while guar gum and PVA are incorporated to improve the material's functional groups, mechanical stability, and adsorption capacity. The prepared composites were employed for the removal of heavy metal ions from aqueous solutions. The prepared composites were characterized by Fourier transform spectroscopy, X-ray diffraction and Scanning electron microscopy. This research will contribute to development of eco-friendly material for wastewater remediation. change this according to new study. The results revealed that PVA composites were mechanically stable and efficient adsorbent with enhanced heavy metal adsorption properties.

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## Synthesis of Guar Gum beads for drug delivery application

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Tramadol is an analgesic that need repetitive administration due to un-controlled release and low bioavailability in the body. In this research work, Guar Gum beads were synthesized by precipitation method for loading Tramadol HCl. The structural confirmation of prepared beads was accomplished by FTIR, SEM and XRD analysis. The swelling studies revealed the pH responsive behaviour of beads and showed the sustained release of the drug up to 12h at pH 7.4 which proved these beads to be effective drug carriers. The prepared samples were biocompatible, biodegradable and cost-effective drug carriers for a variety of analgesic drugs.

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## **Prussian Blue Nanoparticles Photodegradation Activity**

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Prussian blue nanoparticles are used for industrial water treatment having organic dyes like methyl red and methylene blue. A synthetic azo dye methyl red (MR) is widely used in many industries like textile, paper industry, food processing and water treatment, known for its persistent nature and health risks even in very low concentration. Various methods are used to degrade MR including chemical and biological methods. Photo-degradation of methyl red using sawdust supported Prussian blue nanoparticles (SD- PBNPs) has been investigated. Nanoparticles are synthesized by co-precipitation method. The nanoparticles were characterized by using various techniques. The photo-degradation efficiency was evaluated under UV-Vis light irradiation, the results showed that sawdust supported Prussian blue nanoparticles proved to be efficient source for removal of MR. The degradation activity is enhanced due to the larger surface area of the Prussian blue nanoparticles due to adsorption on saw dust. The method proved to be cost effective and ecofriendly. The stability and recyclability of synthesized nanoparticles were also investigated. Results showed that the sawdust supported Prussian blue nanoparticles perform great photo-catalytic activity till five consecutive cycles. Further investigations are required to understand its mechanism.

## Advanced Cu @alpha MnO<sub>2</sub> Coupled with S@g-C<sub>3</sub>N<sub>4</sub>: A Breakthrough in Photoelectrocatalysis for Overall Water Splitting

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Photo electrocatalytic water splitting is a promising and sustainable approach for hydrogen production, offering a clean alternative to fossil fuels. It involves the utilization of light-driven catalysts to efficiently split water into hydrogen and oxygen, contributing significantly to the advancement of renewable energy technologies. In this research project, alpha-manganese dioxide ( $\alpha\text{MnO}_2$ ) nanoparticles were synthesized using a hydrothermal method and subsequently doped with varying percentages of copper (1, 3, 5, 7, and 9 wt.%). To further enhance their catalytic performance, the doped nanoparticles were supported on Sulphur-doped graphitic carbon nitride (SGCN) with varying weight percentages (10, 30, 50, 70, and 90 wt.%). This hybrid nanomaterial was investigated for its application as a photo electrocatalyst in water splitting, as well as its performance in supercapacitor systems. Fluorine-doped tin oxide (FTO) glass substrates were used as working electrodes, which were modified with the synthesized Cu@ $\alpha\text{MnO}_2$ -SGCN nanocomposites. Electrochemical evaluations such as Linear Sweep Voltammetry (LSV) for oxygen and hydrogen evolution reactions (OER, HER), Cyclic Voltammetry (CV), Electrochemical Impedance Spectroscopy (EIS), and Chronopotentiometry were performed to determine the catalytic activity. Among the various compositions studied, the nanocomposite containing 7 wt.% Cu and 50 wt.% SGCN showed the most promising results, suggesting its potential as an efficient photo electrocatalyst for renewable hydrogen generation.



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## **Preparation of Alcohol-Free Royal Musk Spray Perfume: A Simple Method for Creating Natural Fragrance**

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This study describes the preparation of an alcohol-free royal musk spray perfume using essential oils and carrier oils, aimed at creating a gentler, natural alternative to alcohol-based perfumes. The process involves blending royal musk fragrance oil, carrier oils such as jojoba oil or fractionated coconut oil, distilled water, and optional glycerin for enhanced longevity. The resulting product is evaluated for its fragrance intensity, longevity on the skin, and overall sensory profile. The study highlights the benefits of alcohol-free perfumes, which provide a more skin-friendly and environmentally conscious option. The preparation method results in a natural, long-lasting musk fragrance suitable for daily use.

## **Harnessing Cu@Cr<sub>2</sub>O<sub>3</sub> with S@g-C<sub>3</sub>N<sub>4</sub> Nanostructures for Next Generation Water Splitting.**

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Photoelectrochemical (PEC) water splitting offers a sustainable approach to hydrogen production. This research focuses on the synthesis of Cr<sub>2</sub>O<sub>3</sub> nanoparticles by Co-precipitation method. Afterward, these nanoparticles were doped with varying percentages of Cu (1,3,5,7,9 and 11 wt%). 9% Cu@Cr<sub>2</sub>O<sub>3</sub> revealed best photo electrochemical ability for overall water splitting. To further observe and elaborate, the effect of S@g-C<sub>3</sub>N<sub>4</sub> was checked as a substrate material. 9% Cu@Cr<sub>2</sub>O<sub>3</sub> was made composite with varying percentages of S@g-Cr<sub>2</sub>O<sub>3</sub> (20,40,60 and 80 wt%). Outcomes suggested that 60% Cu@Cr<sub>2</sub>O<sub>3</sub> @SGCN was the best electro catalyst. The electrochemical activities for whole water splitting process were monitored by using chronopotentiometry, cyclic voltammetry (CV), linear sweep voltammetry (LSV), and EIS. The electrochemical water splitting of Cu@Cr<sub>2</sub>O<sub>3</sub> @SGCN exhibits maximum performance, resulting in a low over potential for OER and HER, good stability and achieving a higher current density. This work shows the potential of this synthesized nanomaterial as a stable photo catalyst for PEC photoelectrochemical water splitting.

## Exploring Phytochemical-Based Gene Targeting for Bullous Pemphigoid: A Computational Approach

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Bullous pemphigoid is a rare autoimmune skin disorder that causes large, fluid-filled blisters due to the immune system mistakenly attacking skin proteins BP180 and BP230. This process involves autoantibodies triggering inflammation, leading to skin damage. Certain phytochemicals have the potential to target the genes and proteins involved in the disease. Compounds such as curcumin, quercetin, and resveratrol have demonstrated anti-inflammatory and immunomodulatory properties, making them promising candidates for therapeutic intervention. However, no in silico studies have been conducted to explore their specific effects on bullous pemphigoid-related targets. In silico research on phytochemicals could help identify effective treatment options, reducing the need for extensive laboratory testing and accelerating drug discovery.

## Nature Meets Technology: *In-Silico* and Herbal Innovations in Epilepsy Management

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Chronic epilepsy is a medical disorder distinguished by indeterminate, unidentified seizures that originate by erroneous brain impulses and an aberration in the usual functioning of brain cells. The disparity between glutamate and inhibitory transmitters in the brain is the primary root of epilepsy, and this asymmetry is often linked to either lower GABAergic activity or increased glutamatergic activity. The key inhibitory neurotransmitter is gamma-aminobutyric acid (GABA), and the possibility of seizures and heightened neuronal excitability are both directly connected to its crashing. Gamma-aminobutyric acid, or GABA, is the primary inhibitory neurotransmitter in the brain. It interacts by adhering permanently to receptors, predominantly GABAA receptors, which boost chloride conductance into the cell and generate hyperpolarization. Herbal medicines have been employed for centuries for managing epilepsy, and present investigations are looking at evidence from science supporting these long-standing assertions. Findings suggests natural therapies can enhance epilepsy delay and prolong seizure severity in convulsions provoked by strychnine and pentylenetetrazol (PTZ), apparently by regaining GABA levels in the brain and influencing the GABAergic neurotransmitter cascade. With the aim to locate novel the pharmaceutical targets, investigate the mode of activity of newly discovered chemicals, and boost the creation of drugs, in silico studies are growing more and more significant in the realm of epilepsy studying. Generating greater effective and accepted AEDs is one of the prospective focuses of epilepsy studies. This might be addressed by looking at natural products and using in silico algorithms to find and strengthen new GABA-targeting medications.

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## **Preparation and Characterization of Moisture Bath Bombs**

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Bath bombs are becoming increasingly favored as a skincare item intended to elevate the bathing experience through their moisturizing, soothing, and aromatic qualities. This research examines the creation of moisturizing bath bomb tablets made from a mixture of baking soda, citric acid, essential oils, cornstarch, Epsom salt, and carrier oils. The interaction between baking soda and citric acid produces the distinctive fizzing effect, while Epsom salt offers benefits for muscle relaxation. Essential oils and carrier oils enhance hydration and provide aromatherapy effects, whereas cornstarch improves skin-softening properties. A comparative analysis of the components underscores their individual as well as combined impacts on moisturizing and nourishing the skin. The results indicate that bath bombs with added emollients can be a beneficial and pleasurable self-care product for enhancing skin hydration.

## **Enhanced CO<sub>2</sub> Adsorption Capacity and Selectivity of Zn-Cu BDC Bimetallic MOFs Compared to Monometallic MOFs**

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The paper provides a brief outline of the research of Zn and Cu metal centers in Zn/Cu-BTC MOFs shows higher CO<sub>2</sub> adsorption compared to either Zn-BTC or Cu-BTC alone. The bimetallic nature provides more active sites that enhance the ability to adsorb CO<sub>2</sub>. Zn/Cu-BTC mainly shows adsorption of CO<sub>2</sub> through physical adsorption, that is why they store gases like CO, more effectively. Zn/Cu-BTC MOFs can be synthesized by using hydrothermal or solvothermal methods. The morphology and pore structure of Zn/Cu-BTC play crucial role to CO<sub>2</sub> adsorption and penetration. Some characterization techniques like SEM, TEM, and EDS are applied for the effective preparation of the bimetallic MOFs. Zn/Cu-BTC demonstrate higher CO<sub>2</sub>/N<sub>2</sub> adsorption selectivity as compared to Zn-BTC and Cu-BTC. The bimetallic nature of Zn/Cu-BTC improves CO<sub>2</sub> adsorption capacity in MOFs. MOFs have 3-D networks. All MOFs are recognized due to the high porosity and thermal stability and firm structure of the metals with organic ligands. The pore size plays a crucial role in gas-adsorption performance. MOFs can be characterized by using various techniques. Field Emission Scanning Electron Microscopy (FE-SEM) is used to investigate morphology (shape and size) of the materials. phase structure can be investigated by using X-ray Diffraction (XRD). By using Fourier Transform Infrared Spectroscopy (FTIR) we can study Chemical properties of MOFs. The study highlights that zinc-copper BDC bimetallic based MOFs reveal promising abilities for selective gas adsorption. They gain more attention in applications of energy and environmental sectors by exploring various functionalization approaches to additional enhance the performance of these MOFs is also significant. In future more Investigation requires for the long-term stability and recyclability of Zn/Cu-BTC MOFs in real-world applications.

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## **Low Cost and Facile Method for the Preparation of Organic Mosquito Repellent**

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Mosquito-borne illnesses like malaria, dengue, chikungunya, and Zika virus are serious health threats, particularly in tropical and subtropical areas. While many people rely on synthetic repellents like N,N-Diethyl-meta-toluamide (DEET), there are growing concerns about their toxicity, environmental effects, and high prices. This study introduces a simple and cost-effective way to create an organic mosquito repellent using essential oils from plants such as citronella, neem, eucalyptus, and lemongrass. These oils were extracted through steam distillation and mixed into a stable emulsion with ethanol and natural fixatives. The effectiveness of the repellent was tested against *Aedes aegypti* and *Anopheles* mosquitoes, demonstrating significant protection for up to 6 hours. This research showcases a sustainable and budget-friendly method for mosquito repellents, encouraging the use of natural bioactive compounds to help prevent diseases.



Knowledge is in many things and can have many different garbs and can have many different directions and dimensions but the knowledge that is gained by seeking the truth and knowledge that comes out of the pursuit of truth, unbiased, unprejudiced, based upon crystalline reasoning and logical understanding and rational thinking is the one that we care for and we should value. So knowledge is actually consisting of truth and nothing but truth.

(Dr Hasan Sohaib Murad)

