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School of Science



4th UMT INTERNATIONAL CHEMISTRY CONFERENCE ON EMERGING TRENDS IN CHEMISTRY

ABSTRACT BOOK

UMT MULTIDISCIPLINARY SCIENCE CONGRESS 2026

STRENGTHENING INTERDISCIPLINARY RESEARCH TO
DRIVE SCIENTIFIC EXCELLENCE

June 4-6 (Thursday-Saturday), 2026

Organized by
Department of Chemistry
School of Science
University of Management
and Technology, Lahore, Pakistan

PREFACE

The Department of Chemistry, School of Science, University of Management and Technology (UMT), Lahore, Pakistan, organized the 4th International Conference on Emerging Trends in Chemistry (CCUMT-2026), held from June 4-6, 2026, at the 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, the 4th CCUMT-2026 seeks to foster interdisciplinary collaboration, explore innovative methodologies, and address contemporary academic and industrial challenges. The themes were Computational Chemistry, AI in Chemistry, Analytical, Environmental, Green Chemistry, Organic Chemistry, Medicinal Chemistry, Natural Product Chemistry, Inorganic Chemistry, Material Chemistry, Nano Chemistry, Nuclear Chemistry, Applied, Industrial, Polymer, Textile Chemistry, Bio Chemistry, Nutritional Food, Agricultural Chemistry, Physical Chemistry, Radiation Chemistry, and Electrochemistry.

The international speakers from China, Saudi Arabia, Spain, Canada, USA and Turkey attended the conference in hybrid mode, online as well as on campus. A total of 170 participants attended the conference, and a total of 82 research papers were presented related to the conference themes, out of which 45 were oral presentations and 37 were poster presentations from all over Pakistan.

The best part was that students from different universities were able to visit under one roof and interact with renowned national and international scientists. The honorable guests, Dr. Talat Naseer Pasha (Director General – Punjab Agriculture, Food and Drug Authority) and Dr. Kauser Abdullah Malik (President – Pakistan Academy of Sciences), inaugurated the conference.

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

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ORAL PRESENTATIONS

Synthesis and Characterization of Metal-Organic Framework-5 (MOF-5) & Its Hybridization with Humic Acid

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Metal organic frameworks (MOFs) have proven to be versatile and can be used in environmental remediation, catalysis as well as in enhanced material uses by being high surface area, tunable porous and by diverse chemical functionality. MOF-5, made of metal clusters of zinc with terephthalic acid, is the most crystalline and most capable of adsorption, however, it is struggling to cope with issues of functional diversity and environmental stability. Humic acid (HA) is a unsurprisingly occurring organic material that contains carboxyl, hydroxyl and phenolic functional groups and therefore is a promising approach to improving the chemistry and functions of MOFs on their surfaces. MOF-5 was synthesized in this study by a solvothermal process and the solvent was exchanged with ethanol to eliminate the traces of DMF and open up the pores. Powder X-ray diffraction (PXRD) and Fourier-transform infrared spectroscopy (FTIR) were used to characterize the synthesized MOF-5 and determine its high crystalline and phase purity and the successful coordination of Zn^{2+} ions and terephthalate linkers. Humic acid was obtained from coal under natural conditions that coordinated with metals. Then the heterogeneous compound of MOF-5/HA was obtained by adding HA to MOF-5 in an alcoholic solution. The retention of MOF-5 crystalline framework was evident through PXRD and the presence of coordination, hydrogen bonding and surface adsorption interactions between HA functional groups and MOF-5 metal nodes were observed in FTIR spectrums. Associations with MOF-5 structural integrity and reactive functional diversity were merged into a hybrid material with better surface functionality, chemical stability and adsorption potential. The findings revealed that the products of MOF-5/HA composite can be widely applied to resolve the environmental issues.

Mechanochemical Synthesis – A prospective tool for Green Chemistry

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Mechanochemical synthesis has emerged as a transformative and sustainable approach in modern synthetic chemistry, offering an environmentally benign alternative to conventional solution-based methods. This talk highlights the core principles of green chemistry, including atom economy, safer synthesis, reduced toxicity, and energy efficiency of mechanochemistry, emphasizing how mechanical energy can drive chemical reactions with minimal or no solvent consumption, thereby significantly reducing hazardous waste and energy requirements. The performance and potential of mechanochemical synthesis in coordination compounds, pharmaceuticals, metal–organic frameworks, nanomaterials, and bioactive conjugates, demonstrating improved reaction rates, selectivity, and product yields is discussed. Attention is drawn to scalable techniques such as ball milling and twin-screw extrusion, along with their industrial relevance and potential for sustainable manufacturing. The talk further addresses challenges associated with reaction monitoring, mechanistic understanding, reproducibility, and scale-up, while presenting future perspectives for integrating mechanochemistry into academic research and industrial production. The talk positions mechanochemical synthesis as a promising prospective tool capable of advancing green and sustainable chemistry in the twenty-first century.

Managing Diabetes with Novel Drug Discovery: Challenges and Opportunities

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Diabetes mellitus (DM), a chronic and progressive metabolic disease of carbohydrate metabolism, certainly remains one of the most debilitating non-communicable health challenges around the globe. The metabolic disorder is generally characterized by elevated blood glucose levels. According to the International Diabetes Federation, 536.6 million individuals worldwide suffered from type 2 diabetes in 2021, making up around 90% of all occurrences of the disease and is predicted to go up to 783.2 million by 2045. DM severely impacts millions of people worldwide and leads to numerous other serious health problems such as kidney diseases, cardiovascular diseases, obesity, blindness and hypertension adding significant cost to the healthcare system. One of the strategies to manage the hyperglycaemic condition in type 2 patients includes the inhibition of digestion and absorption of dietary carbohydrates. In this perspective, α -glucosidase and α -amylase are the two crucial saccharides hydrolyzing enzymes having an impact on the digestion and breakdown of the carbohydrates. The inhibition of these enzymes has culminated in the implementation of robust prevention programmes in the form of developing effective pharmacological agents with favourable impact on the management of T2DM. The current presentation will highlight some of our recent research efforts in the identification of novel inhibitors of these enzymes showing improved efficacy, potency, and reduced adverse effects thus providing possible future therapeutics to address the challenging diabetic complications.

Edible Oil Processing Industry its Environmental Challenges and Waste Management

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On the one hand, the edible oil processing industry plays a very important role in global food supply chains. While, on the other hand it may be a potential source of environmental issues due to its various waste generation and intensive operations. The main source of waste generation may include large amount of water consumption, effluent discharge containing organic matter, air emissions from boilers, oil residues, and its processing stages generating diverse types of waste materials. Solid wastes such as dust, seed husks, packaging materials, spent bleaching earth may further contribute to environmental challenges. Wrong disposal of these wastage materials can cause to soil, air and water contamination as well as ecological imbalance. Therefore, an effective waste management approaches such as use of energy-efficient technologies, wastewater treatment, proper utilization waste materials, use of waste as an ingredient of useful products, adoption of circular economy practice are important strategies to control or minimize the impacts of waste materials. The viable strategies such as consideration of waste materials as by-products and their use for the production of biofuels, animal feed, or fertilizers that will not only reduce the environmental pollution but also increase resource efficiency and lead to the value addition of the industry.

Key Words: Edible oil processing, Waste material, Environmental challenges, Waste management.

Bio-Based Materials for Industrial Applications

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The growing demand for sustainable materials has catalyzed significant research into biobased materials as viable alternatives to conventional petrochemical-based products. This presentation explores recent advances in the development, characterization, and industrial integration of bio-derived polymers and biomaterials. Emphasis is placed on the synergistic effects of combining bio-based matrices with functional nanomaterials to enhance mechanical strength, thermal stability, barrier properties, and biodegradability. Applications across various sectors including packaging, agriculture, and targeted drug delivery are discussed, highlighting both performance improvements and environmental benefits. Furthermore, challenges such as scalability, cost-effectiveness, and end-of-life management are critically assessed. This talk aims to provide a comprehensive overview of how innovations in green polymer science and nanotechnology are driving the transition toward a more sustainable industrial landscape.

Valorization of Banana Peel Waste into Zr-MOF@AC Composite for Sustainable Methyl Orange Removal from Water with Kinetic, Isothermal and Thermodynamic Insights

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Zr-based metal-organic framework (Zr-MOF) and its composite (Zr-MOF@AC) with activated-carbon (AC) were formed via solvothermal techniques at room temperature using safe solvent water. Activated-carbon prepared from agricultural waste (banana-peels) to utilize this unwanted waste to remove toxic pollutant from water. Both Zr-MOF and its composite were successfully characterized using advance spectroscopic techniques. Fourier Transform Infrared Spectrophotometer analysis confirms the successful formation of both adsorbents due to the functional-groups (Zr-O) peaks at 743cm^{-1} and X-ray Diffraction confirms the degree of crystallinity and phase composition. The external structure, dimension of particles, and chemical breakdown of the produced materials were displayed by Field Emission Scanning Electron Microscopy and Energy Dispersive X-ray and thermal stability were checked using thermogravimetric analysis. The composite gives maximum performance at $\text{pH}=6$ with amount of 0.01g MOF and composite, achieving maximum adsorption capacity up-to 280.08 and 243.9 mg.g^{-1} respectively, within 45 minutes. The best fitted kinetics is pseudo second-order model for Zr-MOF and composite. The Langmuir model is best fitted for the adsorption of the MO on the composite, according to isothermal study. Thermodynamic study shows that reaction is spontaneous and exothermic. This study demonstrates the promise of an inexpensive, environmentally acceptable nanocomposite for the elimination of colours from our surroundings. This study confirms the potential of low-cost, eco-friendly composite for dyes removal from environment.

Keywords: Banana peels, Adsorption study, Water purification, Isothermal and Kinetic study, Metal organic frameworks

Study the Green Synthesis Nanoparticles (GSNPs)-Doped Based Sustainable Display Technology

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This research focuses on the preparation and characterization of multi-functional resins and nanoparticles for smart PDLC (polymer-dispersed liquid crystal) windows. Specifically, it examines systems using epoxy resin monomers, hardeners, thermotropic nematic liquid crystals (NLCs), and Aluminum oxide nanoparticles ($\text{Al}_2\text{O}_3\text{NPs}$) and Silver nanoparticles (AgNPs). The primary objective is to develop efficient smart glass films using a polymerization-induced phase separation (PIPS) heat-curing approach. Aluminum oxide nanoparticles ($\text{Al}_2\text{O}_3\text{NPs}$) are synthesized via the Sol gel method, while Silver nanoparticles (AgNPs) are synthesized by solution method; followed by characterization using X-ray diffraction (XRD) to assess crystal structure, crystallite size, and micro strain. LCD parameters testers and scanning electron microscopy (SEM) further characterize the smart glass thin PDLC film. Interactions among resins, hardeners, catalyst, NLCs, and various Al_2O_3 and AgNPs feed ratios are evaluated with cholesteric liquid crystal device methods. SEM validates the microstructure and LC domain dispersion within the polymer matrix. A to F systems have been prepared with constant weight ratio of liquid crystal and hardener while weight ratio of monomers, catalyst, and nanoparticles vary. The data from electro optical

properties denote that the threshold voltage (V_{th}) and saturation voltage (V_{sat}) raise in both the system (B-C) as the amount of penta functional NDGE resin and nanoparticles increased. The rise time (T_{on}) and decay time (T_{off}) values decrease while contract ratio is increasing. This technology supports the construction of commercial agricultural farms, such as betel-leaf and other UV-sensitive crops. It enables agricultural environments to be tailored for optimal growth conditions. Additionally, switchable smart films can reduce reliance on traditional window treatments by providing energy-efficient, environmentally friendly electric curtains, switchable projection screens, and multifunctional switchable glass applications that integrate touch IR, LED tubes, projectors, and other smart film features.

Keywords: Thermotropic Phase, Intelligent PDLC Films, monomers, Aluminium oxide nanoparticles (Al_2O_3 NPs), Silver nanoparticles (AgNPs), and sustainable technology.

Polymer-Assisted Synthesis of Ternary Magnetic Graphene Oxide Nanocomposite for the Adsorptive Removal of Cr (VI) and Pb (II) Ions

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The presence of chromium [Cr(VI)] and lead [Pb(II)] ions in the water bodies has adverse effects on humans and aquatic life. Graphene oxide-based magnetic nanocomposites synthesized in the presence of chitosan (mGO/CS) or polyaniline (mGO/PA) as potential adsorbents for the removal of Cr(VI) and Pb(II) ions. The FTIR (Fourier transform infrared spectroscopy), EDX (Energy dispersive X-ray), XRD (X-ray diffraction) and SEM (Scanning electron microscopy) were employed to investigate the chemical composition, structural, elemental analysis, crystalline size and morphology of the nanocomposites. The FTIR results confirmed the synthesis of the nanocomposites by detecting peaks of specific functional groups. The average crystallite sizes of the mGO, mGO/CS, and mGO/PA nanocomposites were 17, 25, and 23 (nm), respectively, as determined by the Debye-Scherrer equation from the XRD data. Batch adsorption experiments were conducted for Pb(II) and Cr(VI) removal by varying the variables like pH, concentration of metal ions and contact time. The Box Behnken design (BBD) was used to optimize the adsorption parameters. Under the optimum conditions, mGO/CS and mGO/PA showed maximum removal percentages (%R) of 92.36 and 98.7 for Pb(II), and 85.25 and 93.08 for Cr(VI), respectively. The adsorption capacities were 110.84 and 118.44 mg/g for Pb(II), and 87.74 and 111.7 mg/g for Cr (VI) were obtained for mGO/CS and mGO/PA, respectively. The pseudo-second-order kinetic model and Langmuir isotherm fitted well to the experimental data and explain the adsorption mechanism of the nanocomposite materials for both metal ions.

Exploring Transition Metal Electrocatalysts for Efficient and Green Hydrogen Generation

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The escalating consumption of fossil fuels and their detrimental impact on the environment have necessitated the development of sustainable and carbon-free energy alternatives. Among these, hydrogen has gained considerable attention as a clean and efficient energy carrier, offering a high gravimetric energy density of 120–142 MJ/kg. Electrochemical water splitting has emerged as a promising strategy for hydrogen production. However, the overall efficiency of this process is limited by the inherently sluggish kinetics of the two half-cell reactions involved—namely, the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER)—which demand significant overpotentials to proceed effectively. This limitation underscores the critical need for efficient electrocatalysts.

In recent years, substantial research efforts have been directed toward the development of low-cost and efficient electrocatalysts composed of earth-abundant, non-noble transition metals. In this study, we focus on the synthesis of cost-effective bimetallic transition metal oxide electrocatalysts for enhanced HER and OER performance. Using facile drop-casting and hydrothermal methods, Cu–Co, Ni–Co, and Ni–Cu bimetallic oxides were fabricated directly on fluorine-doped tin oxide (FTO) glass substrates and nickel foam. The synergistic interactions between the bimetallic components, along with controlled morphological modifications, were employed to enhance their catalytic activity. The structural properties of the synthesized electrocatalysts were investigated using various spectroscopic techniques. Electrochemical performance was evaluated using a standard three-electrode setup on an electrochemical workstation/potentiostat. The copper-cobalt bimetallic thin films having metal ratios as Cu:Co (1:5) displayed the lowest onset potential of 130 mV. L-lysine assisted NiCo oxides displayed an over potential of 420 mV for attaining current density of 50 mA/cm². The Ni-Cu prepared at various reaction times, showed 390 mV overpotential value for achieving current density of 10 mA/cm² with 24 hours deposition time. The results demonstrated excellent catalytic activity for both HER and OER, highlighting the potential

of these electrocatalysts in sustainable hydrogen production, with superior efficiency, durability, and environmental compatibility.

Key words: Bimetal Oxides, One-Step Hydrothermal Synthesis, Electrochemical Water Splitting, Binder-free Electrocatalysts, Hydrogen Production.

Synthetic Heterocycles: A Step towards Drug Development for Alzheimer's disease and Various Other Metabolic Disorders

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Alzheimer's disease (AD) is a multifactorial neurodegenerative disorder which is the most integral cause of Dementia involving cognitive decline & most prevalent in elders. It is more common in developed countries e.g. Western Europe, United States compared to Asia and Africa, with substantial numbers of affected individuals in South and East Asian regions, particularly China, Japan & India. But its prevalence is now increasing in Pakistan which is the 6th most populated country in the world having 150-200 thousand people with Dementia. Researchers have observed a 2 - 6% rise in Dementia cases among people over 65 years of age. Same for huge risks for metabolic disorders. The present project aims to unleash the pharmacological profile of 1,2,4-triazole or 1,3,4-oxadiazoles, one of the emerging privileged scaffold along with structure-activity relationship. The comprehensive work which will be carried out on 1,2,4-triazole & 1,3,4-oxadiazoles nucleus will provide inevitable scope for researchers towards advancement of novel potential drug candidates having better efficacy and selectivity. Furthermore, the interaction of various analogues with enzymes active sites and their stability will be evaluated with the help of molecular docking and Density Functional Theory (DFT) results, respectively. The computational approach will provide valuable insights into both the physicochemical and pharmacokinetic properties of these derivatives & will lay foundation for facilitate the experimental studies & potential therapeutic applications. All were characterized, and investigated to unravel their anticholinesterase potential. Synthetic N-(substituted) triazoles are assessed for Alzheimer's disease treatment. Modern spectroscopic techniques were used to characterize all synthesized compounds, and assessments of their structure-activity relationships (SAR) were discussed. In addition, the molecular docking analysis unveil that these compounds have better and more stable interactions with the active site of the enzymes. Overall, all these results reveal that these analogs may aid as dual and potential inhibitors of cholinesterase and other enzymes for treating various disorders. Final aim is In-vivo studies will be a step further towards clinical trials.

Construction of Heterocyclic Thiosemicarbazone Hybrids through Sequential Functionalization and Condensation Strategies

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Thiosemicarbazones are versatile scaffolds in synthetic organic chemistry due to their easy preparation and structural tunability. This work presents the design and synthesis of structurally diverse thiosemicarbazone-based hybrids built around quinoline, piperidine, morpholine and thiophene pharmacophores using practical multistep and microwave-assisted methods. Quinoline thiosemicarbazones were prepared through *N*-acetylation, Vilsmeier-Haack formylation, nucleophilic substitution and final condensation with substituted thiosemicarbazides. On the other hand, morpholine-thiophene hybrids were accessed through isothiocyanate formation, hydrazination and condensation. These approaches enabled broad structural diversification and rapid assembly of target libraries in good to excellent yields, with microwave irradiation reducing key condensation steps to 3-5 min.

All compounds were characterized by FTIR, ¹H NMR, ¹³C NMR, and where applicable, mass spectrometry. Biological evaluation identified potent cholinesterase and urease inhibitors, among these structurally diverse derivatives. Overall, these studies demonstrate the synthetic versatility and medicinal potential of thiosemicarbazone hybridization for developing enzyme-targeted heterocyclic scaffolds.

Keywords: Synthesis, Quinoline, Thiosemicarbazone

Assessment of Various Photothermal Materials for Interfacial Solar Vaporization

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Water scarcity is a serious challenge and causes problems for two billion people worldwide. Applying into solar energy seems to be a viable and sustainable solution for the ongoing global challenges of water scarcity and clean energy shortage. However, low evaporation rates often compromise the natural mechanism of solar energy-driven water evaporation. Therefore, the current study presents use of an interfacial solar evaporator to achieve localized heating on the water vapor-liquid interface by photothermal materials. To develop an Efficient Interfacial Solar evaporator, two types of photothermal materials known as Plasmonic Janus Membrane imprinted with CuO nanoparticles and biochar were prepared and characterized with the help of SEM, BET, FT-IR and UV-visible spectroscopy. These photothermal materials show high activity, contain functional groups with aromatic rings and hydroxyl groups, have a porous structure and large surface area. Interfacial solar evaporator developed during experimental work which contains photothermal material floating on the surface of water and experimental work was done by utilizing normal sunlight. The mass change of water was calculated by using an Electronic Balance and a Thermometer was used to check temperature changes after each hour. It has been found that the temperature increase is highest in Plasmonic Janus Membrane imprinted with CuO nanoparticles than in biochars due to the Surface Plasmon Resonance Effect of CuO nanoparticles. The evaporation rate was compared in which biochar shows highest evaporation rate of 0.433 Kg/m²/h in comparison to CuO imprinted Plasmonic Janus Membrane with 0.347 Kg /m²/h while water without photothermal material shows 0.214 Kg/m²/h evaporation rate. It is concluded that the highest evaporation rate of biochar is due to its hierarchical porous structure and the presence of aromatic functional groups. Hence, biomass-derived interfacial solar evaporation provides a cost-effective solution to water scarcity.

Closing the Carbon Loop: Sustainable Production of Syn Gas from CO₂ by Molecular Catalysts

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The utilization of CO₂ 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 CO₂ into a mixture of CO and H₂ at commercial scale still requires efficient electro catalyst. In this perspective, a series of new palladium complexes¹⁻³ with general formulas, [Pd(L¹)(Y)]Y, [Pd(L²)(Y)₂] and [Pd(L³)(Solvento)] Where L¹⁻³ are different donor flexible spectator ligands and Y/ Solvento are actor ligands, were utilised as active electrocatalysts for the conversion of CO₂ 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 CO₂ interaction with each Pd(II) catalyst. The best electrocatalytic activity for CO₂ 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⁻¹ and 81% FE of CO. These pincer scaffolds can be stereo-chemically tuned with its exploration with earth abundant first row transition metals for further improvement in CO₂ reduction chemistry.

Digital Chemistry: Transforming Molecular Science through Computational Innovation

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Chemistry is undergoing a fundamental transformation as computational innovation reshapes how molecular science is conducted, moving beyond purely experimental traditions toward an integrated digital paradigm. While classical chemistry has provided the empirical foundation for understanding atomic structure, bonding, and reaction mechanisms, it remains constrained by time-intensive procedures, resource demands, safety risks, and the practical impossibility of exploring a chemical space estimated at 10^{60} possible small molecules through trial and error alone. This work examines "Chemistry 4.0," a digital transformation built on automation, digitalization, connectivity, and intelligence, which mirrors the broader Industry 4.0 movement by embedding robotics, cloud infrastructure, and AI-driven analysis into chemical workflows.

Central to this shift is digital chemistry itself: the application of computational methods, data science, and artificial intelligence to predict and design chemical systems through molecular modeling, cheminformatics, and machine learning. Key enabling technologies discussed include deep learning architectures such as convolutional, recurrent, graph, and transformer networks for molecular property prediction and retrosynthesis planning; quantum computing approaches like the Variational Quantum Eigensolver and Quantum Phase Estimation for simulating inherently quantum molecular systems; and molecular dynamics simulations for capturing time-dependent behavior such as protein folding and drug binding.

The presentation also addresses persistent challenges, including data quality and availability, model interpretability, current limitations in quantum hardware, and the need for interdisciplinary training that bridges chemistry and computational science. It concludes that realizing digital chemistry's full potential requires sustained investment in computational infrastructure, open data practices, and collaborative training, positioning computational innovation not as a replacement for experimental rigor but as its essential complement in accelerating discovery across medicine, materials, and sustainability.

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.

Recovering Heavy Metals from Electroplating Wastewater and Their Conversion into Zn₂Cr- Layered Double Hydroxide (LDH) for Pyrophosphate Removal from Industrial Wastewater

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This work incorporated technological values into Zn₂Cr-layered double hydroxide (LDH), synthesized from unused resources, for removal of pyrophosphate (PP) in electroplating wastewater. To adopt a resource recovery for the remediation of the aquatic environment, the Zn₂Cr-LDH was fabricated by co-precipitation from concentrated metals of plating waste that remained as industrial by-products from metal finishing processes. To examine its applicability for water treatment, batch experiments were conducted at optimum M²⁺/M³⁺, pH, reaction time, and temperature. To understand the adsorption mechanisms of the PP by the adsorbent, the Zn₂Cr-LDH was characterized using Brunauer-Emmett-Teller (BET), X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy/energy dispersive X-ray spectroscopy (SEM/EDS), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS) analyses before and after adsorption treatment. An almost complete PP removal was attained by the Zn₂Cr-LDH at optimized conditions: 50 mg/L of PP, 1 g/L of adsorbent, pH 6, and 6 h of reaction. Ion exchange controlled the PP removal by the adsorbent at acidic conditions. The PP removal well fitted a pseudo-second-order kinetics and/or the Langmuir isotherm model with 79 mg/g of PP adsorption capacity. The spent Zn₂Cr-LDH was regenerated with NaOH with 86% of efficiency for the first cycle. The treated effluents could comply with the discharge limit of <1 mg/L. Overall, the use of the Zn₂Cr-LDH as a low-cost adsorbent for wastewater treatment has contributed to national policy that promotes a zero- waste approach for a circular economy (CE) through a resource recovery paradigm.

Smart, and Sustainable Materials for Electrochemical Energy Storage Devices

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Smart and sustainable materials are playing a pivotal role in advancing electrochemical energy storage devices by combining high performance with environmental responsibility. These materials exhibit intelligent functionalities such as self-healing, adaptability, and responsiveness to external stimuli, which enhance electrochemical stability, safety, and durability. Recent developments focus on nanostructured materials, including transition metal oxides, sulfides, conductive polymers, and carbon-based frameworks, offering high surface area, improved conductivity, and efficient charge storage. In parallel, sustainable approaches emphasize the use of abundant, non-toxic, and recyclable resources, along with green synthesis methods that reduce environmental impact. The integration of these materials into batteries, supercapacitors, and hybrid systems has led to notable improvements in energy density, power density, and cycling stability. Smart hybrid composites and bio-derived materials further contribute to extended device lifespan and cost-effectiveness. Additionally, their application in solid-state and flexible devices supports emerging technologies such as wearable electronics and large-scale energy storage. Despite challenges in scalability and interfacial optimization, smart and sustainable materials provide a promising pathway toward efficient, eco-friendly energy storage solutions that align with global sustainability goals.

Keywords: Smart Matreials; Supercaapcitors; Electrode design; Batteries; Electrolyte

The Multivariate Advantage: Deciphering Complex Chemical Interactions through Design of Experiments (DoE)

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Traditional One-Factor-at-a-Time (OFAT), are often labour and resource-intensive and statistically blind to the complex interactions between process variables. By employing Design of Experiments (DoE), maximum information can be extracted from a minimum number of experimental runs, quantifying not just main effects also the interactions between factors that OFAT methods invariably miss. In the talk, Plackett-Burman Designs (PBD) will be discussed for efficiently screening the most important variables from the many variable. This will be followed into Response Surface Methodology (RSM), specifically comparing the geometric and practical applications of Central Composite Design (CCD) versus Face-Centered Composite Design (FCCD) for modelling process curvature and locating the optimum. Finally, the lecture will demonstrate how these statistical tools integrate into the Quality by Design (QbD) framework. Real-world case studies will be presented to show the advantages of using statistical designs for optimization of the synthesis parameter, robustness and optimization of various HPLC methods.

Keywords: Design of Experiments (DoE), Response Surface Methodology (RSM), Plackett-Burman Design, Central Composite Design, Quality by Design (QbD), Process Optimization.

Sensitive Voltammetric Detection of Non-Steroidal Anti-Inflammatory Drugs at Carbon Electrodes

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The large-scale utilization and improper discarding of pharmaceutical drugs can cause constant accumulation in the environment and living bodies, presenting substantial ecological and public health concerns. Among the wide variety of pharmaceutical contaminants, non-steroidal anti-inflammatory drugs (NSAIDs) are increasingly detected across diverse samples due to their widespread use and stability. Therefore, the development of sensitive, fast, and cost-effective analytical methods for the detection of NSAIDs has become the primary focus of ecological and clinical analysis. In the current study, a graphite pencil electrode was employed for the sensitive detection of an NSAID, Piroxicam. The electrode surface was electrochemically treated in basic solution, which resulted in higher electron transfer kinetics and improved electroactive surface characteristics. The electrochemically pretreated graphite surfaces showed a linear range from 0.03 – 125 μM with a low detection limit and high reproducibility. The developed graphite electrodes were used to assess the Piroxicam in artificial serum, urine samples, and pharmaceutical formulation with adequate results. The developed simple, low-cost, eco-friendly transducer demonstrates the strong potential for pharmaceutical quality control, clinical diagnostics, and environmental monitoring applications.

Innovative Fe-F co-Doped NiO Nanoarrays: Pioneering High-Efficiency Electrochemical Nitrate Reduction to Ammonia

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An efficient and long-lasting electrocatalyst was created for the electrocatalytic NITRR (nitrate reduction reaction) through a well-controlled hydrothermal process, followed by annealing. The catalyst consists of Fe, F-co-doped nickel oxide nano-arrays (Fe-F-NiO NNAs) uniformly prepared to offer high conductivity and many active sites for efficient nitrate-to-ammonia conversion. The analysis results verified the synthesis of the nanostructured Fe-F-NiO NNAs and demonstrated synergy attributed to the mutual contribution of Fe and F co-doping. Fe doping enhances the transfer of charges and active site density, resulting in an effective ion interface and reduced energy barriers. In contrast, F doping promotes the binding of intermediates and facilitates the final desorption of the product. The synergistic effects are reflected in the enhanced selectivity up to 99.9 % and efficiency in ammonia synthesis during the nitrate reduction reaction (NITRR), yielding 20.9 mmol/h.cm² of NH₃ and a Faradaic efficiency of 82.5 % under an applied potential of −1.198 V vs. RHE. Furthermore, the Fe-F-NiO NNAs showed an extended stability (36 h). Isotope tracer experiments ensured that the sensed ammonia exclusively resulted from nitrate reduction. The fabricated Fe-F-NiO NNAs functioned as a capable electrocatalyst for purifying nitrate-laden wastewater, enabling efficient NH₃ extraction.

Nanomaterials for Sustainable Industrial Applications: Emerging Innovations and Key Challenges

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Nanomaterials have been applied in many industries because their physical, electrical, and chemical properties can be tailored for specific uses. They have found roles in wastewater treatment, energy storage, catalysis, coatings, electronics, healthcare, and sustainable manufacturing. In recent years, more focus has been placed on green and scalable synthesis methods that reduce environmental risks and support sustainable practices.

In this work, more than 70 graphene-based nanocomposites were prepared by combining graphene oxide and reduced graphene oxide with transition and non-transition metals. Eco-friendly methods were used, relying on plant extracts and microbial agents as reducing and stabilizing agents. These nanocomposites were tested for their ability to solve industrial problems, particularly in breaking down pollutants from textile, pharmaceutical, pesticide, fertilizer, and chemical industries. Functionalization with metals and metal oxides was shown to improve their catalytic and adsorption performance.

Opportunities for innovation were observed in applying such nanomaterials to industrial systems, including water purification, protective coatings, and cleaner catalytic processes. At the same time, important challenges were identified, such as scaling up production, ensuring safety, meeting regulatory requirements, and moving toward commercialization. Overall, the results showed that nanomaterials could play a key role in driving industrial innovation while also protecting the environment and supporting sustainable development.

Therapeutic Potential of Thymus Linearis in Alloxan-Induced Diabetic Mice: LC-MS Profiling, Biochemical, Histological, and Computational Approaches

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Diabetes mellitus is a metabolic syndrome prone to oxidative stress and often characterized with augmented blood glycemic levels. This study is designed for investigation of in vitro/ in vivo antidiabetic potency of Thymus linearis leave extract along with its metabolic profiling with the help of liquid chromatography/mass spectrometry (LC/MS). LC/MS profiling led to identify four important phytochemicals as myricetin-3-(6-acetylgalactoside), phloridzinyl glucoside, cadaverine, and dicaffeoyl-maloyl-succinoylquinic acid. In vitro assay (α -amylase and α -glucosidase assays) showed IC₅₀ of 402.30 and 371.71 μ g/mL as compared to acarbose (335.04 and 312.86 μ g/mL) respectively. Acute and subacute toxicity analysis showed no antagonistic effects at various doses (250, 500, and 1000 mg per kg of mice body weight). Oral glucose tolerance test (OGTT) in mice showed remarkable decline of blood glucose level in mice treated with extract. During this study, diabetic mice were treated with leave extract of Thymus linearis (250, 500, and 750 mg/kg) for 30 days which significantly lowered the fasting and random blood glucose levels (BGLs) with promoted pancreatic cell regeneration and insulin production. Molecular docking of LC-MS identified phytochemicals with sulfonyl urease, glucagon-like peptide-1, α -amylase, and α -glucosidase receptor proteins showed substantial binding scores along with diverse physicochemical, pharmacokinetic, and toxicological profiles.

Multi-Plant Oil Microemulsion for Hair Follicle Restoration and Scalp Health Enhancement

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Some of the most common dermatological and cosmetic effects of oxidative stress, hormonal imbalance, and inflammation include hair loss and follicular degeneration. The traditional methods of treatment could be rather ineffective and may have side effects, which is why natural and multibioactive preparations need to be used. The paper presents the preparation and initial testing of a multi-oil hydro oil microemulsion serum of Aloe vera gel, pumpkin seed oil, grape seed oil, fenugreek oil, flaxseed oil, pomegranate oil and Ginseng oil to repair hair follicles and improve the health of the scalp. Aloe vera gel was used as the hydrophilic base, and the botanical oils of choice were used as the dispersed lipid phase to prepare a stable oil-gel microemulsion. Physicochemical characterization showed that it had a pH of 5.8 ± 0.2 , viscosity of 72 ± 5 cP and a stable droplet size distribution (average, 180 ± 15 nm) in four weeks at room temperature. In DPPH tests, the serum had an antioxidant activity of 85% and proof of effective free radical scavenging capacity. Initial in vitro experiments with dermal papilla cells showed that there was an increase in cell proliferation of 25% after 48 hours compared to controls which hints to possible follicular stimulation. The botanical activities had synergistic effects in reducing 5-alpha reductase activity by pumpkin seed oil (by 18 percent), microvascular mimic models by grape seed oil, and dermal papilla cell viability by ginseng oil. Fenugreek, flax seed and pomegranate oils are added to the effect of additional anti-inflammatory and barrier-supportive effects. These findings show that the developed serum acts on several mechanisms, which are antioxidant protection, follicular stimulation, and scalp nourishment, to promote hair follicle regeneration. This paper presents a multi-bioactive cosmeceutical platform based on scientific foundations, and the follow-up research will be conducted on in vivo analysis and clinical trials to confirm the effectiveness and discuss the application in the commercial sphere in terms of natural hair care products.

Keywords: Microemulsion of multi-plant oil, Cosmetic follicle regeneration.

Tailoring Drug-Mediated Copper Oxide Nanoparticles with Acetic Acid Capping for Enhanced Colorimetric Oxalic Acid Detection

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The development of kidney stones and, ultimately, chronic renal failure is linked to hyperoxaluria. However, the risk of cardiovascular pathology may be further increased by their elevated levels in blood plasma as a result of renal failure. Therefore, the development of such methods to quickly and affordably detect and quantify oxalic acid is prompted by the global health problem. Therefore, colorimetric sensors that detect oxalates quickly and affordably can be developed using nanotechnology. The intrinsic color change of copper oxide nanoparticles (CuO NPs) increases their significance. The developed paracetamol-mediated CuO NPs were capped with acetic acid and characterized through UV–visible spectroscopy, FTIR, XPS, XRD and SEM, to confirm the synthesis of NPs. CuO NP synthesis was verified by UV-visible spectroscopy using surface plasmon resonance at 225 nm. The stretching vibration of Cu-O in CuO NPs was represented by the peak at 850 cm⁻¹. The spherical shape and particle size of 27.51 nm were verified by the XRD and SEM characterization. Both spectroscopy and the unaided eye revealed the intrinsic colorimetric characteristics of CuO NPs, with a reduction in the blue hue as the oxalate concentration was increased. The developed probe successfully identified oxalate levels in concentrations ranging from 1 to 120 μM with a limit of detection of 0.23 μM and quantification of 0.78 μM. The spiking levels in real samples demonstrated that the developed sensors can be utilized for detecting oxalate in the urine of patients with kidney stones. The developed CuO NPs have shown rapid and precise selective oxalate detection in a linear range. The biosensor offers a great platform for measuring oxalate, which is essential for identifying hyperoxaluria and preventing the development of calcium oxalate stones in the kidneys by using efficient treatment methods.

Synergistic Efficacy of NiCoMn-LDH/g-C₃N₄ Nanocomposite for Enhanced Oxygen Evolution Reaction

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The advancement of sustainable energy conversion technologies depends on the development of effective and affordable electrocatalyst for oxygen evolution reaction (OER). As order to take advantage of synergistic effects for improved catalytic performance, a novel NiCoMn-layered double hydroxide (NiCoMn-LDH) / graphitic carbon nitride g-C₃N₄ nanocomposite was successfully analyzed. Fourier transform infrared spectroscopy-FTIR, Xray diffraction-XRD technique, scanning electron microscopy (SEM), and energy dispersive X-ray spectroscopy- EDX were utilized to systematically differentiate the structural, morphologic, and compositional attributes of the prepared nanocomposite, confirming successful composite formation, uniform dispersion of NiCoMn-LDH nanosheets related the g-C₃N₄ matrix, and intended elemental composition. The NiCoMn- LDH/ g-C₃N₄ nanocomposite has a low-level over-potential of 285 mV at 10 mA cm⁻² and a Tafel slope of 75 mV dec⁻¹, indicating effective charge transfer kinetics and superior OER activity, as determined by electrochemical measurements. Additionally, after extended electrolysis, the catalyst shows outstanding operational stability. The improved performance is evaluate to the synergetic fundamental interaction between the conductive g-C₃N₄ support and trimetallic LDH, which enhances electrical conductivity, increases the compactness of progressive sites, and speeds up the dynamics of oxygen evolution. The rational design of sophisticated hybrid electrocatalysts for effective water splitting and renewable energy applications is made possible by this work.

Keywords: Hydrothermal synthesis, Electrocatalyst, Synergistic behavior, OER

Senary High-Entropy Alkoxides: Overcoming Kinetic Barriers in the Oxygen Evolution Reaction

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High-entropy materials (HEMs) have emerged as a transformative frontier in electrocatalysis, offering unprecedented control over electronic states via extreme compositional complexity. In this work, we report the rational design and synthesis of a senary FeCoNiMoMnCu-alkoxide high-entropy electrocatalyst, uniformly anchored onto acid-activated nickel foam via a scalable deposition strategy. The integration of six distinct transition metals into a single-phase framework induces significant entropy-driven stabilization and pronounced lattice distortion, which collectively modulate the local electronic configuration. Advanced structural and morphological analyses reveal a hierarchical surface architecture that provides a high density of coordinatively unsaturated active sites and facilitates rapid mass transport during gas evolution. Electrochemical evaluations demonstrate that the synergistic interplay between the multi-metal species optimizes the adsorption energies of oxygenated intermediates, thereby effectively lowering the rate-limiting kinetic barriers. Consequently, the catalyst delivers a superior oxygen evolution reaction (OER) performance, characterized by a low overpotential of 258 mV at 10 mA cm⁻², a refined Tafel slope of 48.38 mV/dec, and high turnover frequencies. Notably, the system exhibits exceptional operational durability and structural integrity over prolonged electrolysis, attributed to beneficial in situ surface reconstruction. These findings underscore the potential of entropy-mediated electronic tuning in the development of non-noble-metal systems, providing a robust roadmap for architecting highly efficient and durable electrocatalysts for large-scale sustainable water splitting applications.

Key words: High-entropy materials, Oxygen evolution reaction, Electronic modulation, Surface reconstruction.

Chemical Profiling and Bioactivity Analysis of Metabolites Derived from *Aspergillus Flavus*

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The purpose of this research study was to analyze the biological activities of metabolites from the filamentous fungus *Aspergillus flavus*. FTIR and UV-visible spectroscopy confirmed the presence of functional groups characteristic of pharmacologically active compounds. The EA extract of *A. flavus* contains total flavonoids (3.59 ± 0.02 mg CE/g) and total phenolics (3.017 ± 0.05 mg GAE/g). Twenty biologically active compounds were found using GC-MS analysis. Secondary metabolites of *A. flavus* showed good antimicrobial and antifungal properties, as confirmed by antibacterial and antifungal assays. The sample exhibits good antioxidant properties, as confirmed by the DPPH method, with a scavenging ability of 23.66-84.85%. When tested for cytotoxicity against 3T3 fibroblast cell lines, the extract exhibited low cytotoxicity. Also, molecular docking studies were performed against DNA gyrase and the LasI quorum-sensing proteins.

The Ai Dependency Paradox; Behavioral Impact among Students

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The rapid integration of artificial intelligence into higher education has fundamentally altered the landscape of student learning, raising questions about its long-term effects on cognitive development, academic integrity, and psychological well-being. While AI tools undeniably make complex material more accessible and help reduce cognitive overload, this paper argues that overreliance on such technologies carries significant risks that educators can no longer afford to overlook. Using a combined qualitative and quantitative approach, collecting survey data and student reflections, this study finds that excessive AI usage is closely tied to declining intrinsic motivation and the gradual erosion of core academic competencies, including critical inquiry, analytical reasoning, and reflective revision. Beyond academics, students increasingly reveal adverse psychological effects such as digital exhaustion and a reduced capacity of independent learning. The study also reveals how AI complicates established concepts of originality, generating integrity challenges that surpass traditional definitions of plagiarism. Significantly, the findings reveal that these outcomes are not inevitable. The degree of harm or benefit depends largely on how institutions frame AI use through policy and pedagogy. When thoughtfully integrated, AI can genuinely complement human thinking rather than displace it. The paper concludes with a practical roadmap for educators, centering on two urgent priorities: redesigning assessments to reward authentic intellectual effort, and embedding AI-literacy programs into curricula. The ultimate goal is not to resist technological progress, but to ensure that students entering an AI-saturated world remain confident, independent, and creative thinkers in their own right.

Visible-Light-Driven CO₂ Conversion into Value-Added Fuels Using Metal-Integrated UiO-66-NH₂-SH MOFs

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Photocatalytic conversion of CO₂ into value-added fuels represents a promising and sustainable approach for mitigating global warming while simultaneously addressing growing energy demands. However, low conversion efficiency and poor product selectivity continue to limit practical applications. In this work, rationally engineered metal–organic frameworks (MOFs), denoted as UiO-66-NH₂-SH@M (M = Cu, Fe, Co, Ag, and Au), were developed as efficient photocatalysts for visible-light-driven CO₂ reduction into valuable products such as syngas (CO + H₂), methanol (CH₃OH), and ethanol (C₂H₅OH). The synergistic integration of amine (–NH₂) and thiol (–SH) functional groups, combined with catalytically active metal sites, significantly enhances CO₂ adsorption and activation while improving charge separation and transfer efficiency. Structural characterization using XRD and FTIR confirms the high crystallinity and excellent stability of the synthesized catalysts, whereas UV–Vis diffuse reflectance spectroscopy (DRS) demonstrates enhanced visible-light absorption capabilities. Furthermore, electronic structure investigations through XPS and Mott–Schottky analyses indicate favorable band alignment for photocatalytic CO₂ reduction. Among the synthesized materials, the optimized UiO-66-NH₂-SH@M systems exhibit significantly enhanced solar-driven CO₂ conversion performance compared with pristine UiO-66 frameworks, achieving efficient production of syngas, methanol, and ethanol. Electron paramagnetic resonance (EPR) studies and density functional theory (DFT) calculations further reveal that surface functionalization and metal incorporation promote the formation and stabilization of crucial reaction intermediates, such as CO* and CHO*, thereby directing product selectivity toward liquid fuels. Overall, this study highlights the critical importance of multifunctional modification and atomic-level engineering in MOF-based photocatalysts, offering new insights into the design of highly efficient and selective systems for sustainable solar-driven CO₂ conversion.

Ultra-Processed Food Consumption and Mental Health in adolescents: A NOVA-Based Psychological Assessment Study

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The increasing mental health disorders among adolescents is a significant global concern for public health. Multiple lifestyle factors along with dietary habits like consumption of ultra-processed food and academic stress are increasingly being emerged as reasons behind psychological distress. NOVA classification system demonstrates that UPFs include products that are manufactured industrially such as fast foods, packaged snacks, instant meals, and sugary beverages. These products are typically rich in unhealthy fats, additives and refined sugars but lack most needed essential nutrients. Meta analyses and large-scale systematic reviews provides evidence about consistent association between increased risk of depression and high intake of ultra-processed foods. Moreover, emerging knowledge links greater consumption of UFPs and higher levels of psychological distress, thus indicates a dose-response relationship. Recent studies have also highlighted biological and behavioral pathways that associate UPFs consumption with anxiety and bad mental health outcomes. Such products are a source of increased systemic inflammation, dysregulation of hypothalamic–pituitary–adrenal (HPA) axis, and oxidative stress, all of which are attributable to depression. Furthermore, UPFs may have a negative impact on gut microbiota, in this way, gut-brain axis is disrupted. This leads to reward system over activation and addictive-like eating patterns, which add to poor dietary choices in future as well.

These findings support the growing agreement in nutritional psychiatry that the quality of our diet significantly affects mental health outcomes. This is especially important for young adults facing high levels of academic and environmental stress.

Sustainable Fabrication of Cu-Doped Cadmium Sulfide Nanoparticles for Detoxification of Methyl Blue Dye from Wastewater via Adsorption and Photocatalysis

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This study explores the Methyl blue detoxification through Cu-CdS NPs (Copper-doped Cadmium Sulfide Nanoparticles) via hydrothermal process. These nanoparticles were characterization using UV-Vis spectroscopy, FTIR, X-ray Diffraction, Scanning Electron Microscope and EDX to demonstrate the absorption study, conformation of functional groups, crystal structure elemental analysis, and surface morphology. The Cu-doping approach enhanced the energy gap (E_g) from 2.63 to 3.33 eV as compared to typical CdS NPs which have energy gap (E_g) of $\sim 2.4\text{--}2.8$ eV. This energy band structure modification boosts the charge separation and helps to optimize the photocatalytic activity. The system attained a remarkable photodegradation (96.76 %) of methyl blue dye under adjusted conditions such as 10 μM dye, 2 mg catalyst, and pH (11), which substantially overcome various reported yields. The cost-effectiveness, reduced catalyst dose, and kinetic analysis complied with a pseudo-first-order reaction ($k = 0.046 \text{ min}^{-1}$), which strengthen the reliability of Cu-CdS NPs for commercial deployment. Above all, the present work targets the non-biodegradable and environmentally hazardous dye methyl blue, whose industrial effluents exhibits more extensive complications than methylene blue, forming their decontamination is of significant importance. Furthermore, the outstanding photocatalytic performance in this work

enables eco-friendly synthesis, reinforcing the importance of band gap fabrication, sustainable trajectory to wastewater remediation, surface tailoring, establishing the link between laboratory and industries, along with improved stability and reusability of the Cu-CdS catalyst, demonstrates its promising applicability in wastewater treatment, and market-relevant photocatalyst.

Harmful Effects of Food Preservative BHT on Human Health

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Food preservatives are widely used to extend shelf life, prevent spoilage, and maintain the quality of food products. Synthetic antioxidants such as Butylated Hydroxytoluene (BHT) play a crucial role in delaying oxidation in fat-containing foods. Despite its effectiveness, concerns about its safety have raised questions regarding its impact on human health. This study evaluates the effectiveness of preservatives in increasing food shelf life, focusing on BHT, and assesses its potential health effects. A review-based methodology was adopted, analyzing previous research studies, toxicological data, and reports from food safety authorities. Findings indicate that BHT effectively prevents oxidative rancidity, preserving taste, color, and nutritional value in processed foods such as snacks, oils, and cereals. Although regulatory agencies approve its use within permissible limits, animal studies suggest possible toxic effects at high doses, while human evidence remains limited. A key research gap is the lack of long-term human studies on cumulative exposure. To address these concerns, emerging approaches such as nanoencapsulation of BHT for controlled release, reduction of dosage through synergistic use with natural antioxidants (e.g., plant polyphenols), and replacement with safer bio-preservatives are being explored. These methods aim to minimize potential health risks while maintaining preservation efficiency. In conclusion, while BHT significantly enhances food stability and reduces waste, adopting advanced delivery systems and alternative preservation strategies can improve safety and support better public health outcomes.

Keywords: Food preservatives, Shelf life, Butylated Hydroxytoluene (BHT), Oxidative stability, Human health, Toxicity, Nanoencapsulation, Natural antioxidants, Food safety, Bio-preservatives.

Application of Green Synthesized Zinc Oxide Nanoparticles from Banana and Onion Peels as Antimicrobial Coating Agent for Poultry Meat Preservation

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Meat spoils rapidly due to microbial growth and oxidation, and the limitations of synthetic preservatives highlight the need for safer, eco-friendly preservation strategies. Green-synthesized nanoparticles derived from agro-waste offer a sustainable alternative for improving meat quality and shelf life. This study investigates the green synthesis of zinc oxide nanoparticles (ZnO NPs) using banana and onion peel extracts and their application in chitosan-based edible coatings to enhance the shelf life and quality of chicken meat during refrigerated storage. ZnO NPs were synthesized using agro-waste extracts and characterized through UV-Vis spectroscopy, FTIR, XRD, SEM with EDX, DPPH, FRAP, and antimicrobial assays. The nanoparticles showed a distinct UV-Vis absorption peak at 365-380 nm with a band gap of 3.2-3.3 eV, while FTIR confirmed polyphenolic functional groups aiding nanoparticle stabilization. XRD patterns showed strong crystallinity, and SEM with EDX revealed spherical nanoparticles sized 40-70 nm with high elemental purity. Antioxidant assays indicated high activity, with DPPH scavenging increasing from 20% to 78%, and FRAP values falling within 0.18-0.26 mmol Fe²⁺/g, demonstrating acceptable reducing potential. Antimicrobial activity produced clear inhibition zones of 18-22 mm against foodborne pathogens. When applied to meat, the ZnO-NP enriched chitosan coating-maintained pH at 5.6-5.8, reduced drip loss from 6.2% (control) to 3.1%, preserved color brightness (higher L* and a* values), and slowed texture deterioration by reducing hardness loss by 35%. Uncoated meat spoiled by day 6, whereas coated samples remained acceptable up to day 12, confirming significant improvement in oxidative stability, microbial inhibition, and physicochemical quality. This approach offers a sustainable, low-cost, and highly effective method for meat preservation using agro-waste valorization.

Comparing the Effects of Organic and Chemical Supplementation on Mushroom Growth Dynamics under Resource-Limited Cultivation Conditions

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Mushroom cultivation is a growing field in Pakistan, highlighting its importance as a food product gaining popularity among the population. This study evaluated the effects of organic and chemical supplementation on important mushroom growth dynamics. This study established three groups of *Pleurotus ostreatus* in duplicate in Punjab's spring climate: a control group with base rice substrate only, an organic supplementation group containing 5% wheat bran, and a chemical supplementation group treated with 1% calcium carbonate. The inoculation was performed on 16 March, and it was monitored until 5 April. For inoculation, the substrate was pasteurized by soaking in water at 65°C for 15 minutes. After straining, the damp substrate was filled and sealed in 6 plastic bags for the study. The groups were left in dark conditions for 10 days until maximum colonization was achieved. On the 10th day, 3 cm cuts were made at 10 visually evenly distributed spots on the bags. On the 11th day, pin formation was first observed in the CaCO₃ (1) group, leading to growth spurts in all groups in succession.

Daily growth progression was observed through observational and morphometric analysis. The quantitative parameters assessed include cluster count, pinhead count, fruiting-body count, mature-mushroom count, fresh-harvest weight, edible biomass, stipe height, cap diameter, and daily environmental temperature. Due to high pin density, pin counts were estimated using the quadrant sampling method, and for morphometric measurements, three representative fruiting structures were selected from one representative cluster per group. For classifying developmental stages, morphological observations were made visually. Undifferentiated nodular primordia lacking cap differentiation were labeled pinheads; structures exhibiting initial cap and stipe development were identified as fruiting bodies. Whereas fully developed structures with expanded caps before sporulation counted as mushrooms. The mature mushrooms were then harvested based

on visual indicators of maturity (cap expansion with curvature and absence of visible spores). The analysis showed variations in certain areas dependent on treatment received. CaCO_3 groups showed the densest clustering with rapid development and the highest growth rate generating the most biomass. Bran groups showed a promising yield as well, but comparatively slower growth efficiency. Control groups showed a low- to-moderate status of the parameters. These findings show that meaningful cultivation data can be obtained even in resource-limited conditions if systematic observations are applied. Insightful data were obtained through this study that can be strategically applied to small-scale mushroom cultivation farms.

Integrating RNA-Seq Transcriptomics and Non-Invasive Clinical Indices to Elucidate Shared Fibrotic Pathways in Hepatitis B and C Infections

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Chronic Hepatitis B (HBV) and C (HCV) infections are chronic health issues worldwide that slowly progress to liver fibrosis, cirrhosis and hepatocellular carcinoma. Liver biopsy is the diagnostic reference test for staging, but is very invasive and very expensive. Non-invasive fibrosis scoring systems such as AST/ALT ratio (AAR), APRI and FIB-4 are simple surrogates for fibrosis, but their molecular mechanisms are not well understood. The use of high throughput bioinformatics analysis of these clinical indices can identify shared pathways of viral liver injury. The main goal of this study is to find common differentially expressed genes (DEGs) of HBV and HCV from publically available RNA-Seq data from Gene Expression Omnibus (GEO). In addition, functional enrichment analysis will be conducted in order to find the biological processes that are associated with the increasing levels of clinical markers of fibrosis among these common DEGs. The approach: HBV, HCV and healthy control public RNA sequencing data will be downloaded from the NCBI GEO database. The disease groups will then be compared against healthy controls using the GEO2R analyzer tool, to identify the statistically significant DEGs. Then, functional annotations and pathway mapping of the intersecting DEGs will be carried out by using online tools such as Enrichr or DAVID. Following enrichment analysis, the STRING database will be used to construct and analyze a Protein-Protein Interaction (PPI) network to identify interconnected functional groups. The pathways expected to be highly enriched in the common DEGs are pathways involved in extracellular matrix (ECM) organization and pro-inflammatory cytokine signaling. Specific core platform hub genes such as CCL2 or COL1A1 will give a clear molecular explanation for the clinical decline in platelet counts and the increase in AST/ALT ratios seen in the more advanced fibrosis. Furthermore, network topology analysis will determine whether a single critical gene or a cluster of interconnected hub genes drives disease progression, highlighting key targets for potential therapeutic studies. After summarizing the results, the study provides evidence that common pathogenic mechanisms exist among viral hepatitis, by relating high-throughput transcriptomic data to clinical measures. The results will add

to the understanding of the progression of the virus and help identify potential non-invasive markers and/or novel targets for therapy to stop fibrosis getting worse and developing into cirrhosis.

Strategies to Disrupt Biofilms in Multidrug Resistant Bacterial Infections

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Many bacteria are able to form biofilms which can cause multidrug-resistant (MDR) bacterial infections, a serious global health problem. Biofilms are clusters of bacteria enveloped in a protective layer of exopolysaccharides (EPS) comprised of sugars, proteins, lipids and DNA. This layer provides protection against antibiotics and the immune system, so infections can become persistent and hard to treat. This makes it difficult for normal antibiotics to work, as the bacteria inside biofilms is less active than those in the free environment and there are extremely tolerant persisted cells. This study summarizes the various methods for disrupting biofilms in MDR infections. Biofilm matrix is degraded by Enzymes (DNases and proteases) which facilitate the action of antibiotics. Quorum sensing inhibitors (QSIs) disrupt bacterial communication and inhibit the development of biofilm and severity of infection. Antimicrobial peptides (AMPs) disrupt bacterial membrane and contribute the weakening of the structure of biofilm. The specific targeting and killing of bacteria in the interior of the biofilm while the engineered and CRISPR modified phages penetrate the interior of biofilms is termed as bacteriophage therapy. The use of systems based on nanotechnology, like the use of metal Nanoparticles and drug carriers, enhances the drug delivery and the antimicrobial activity of drugs in biofilms. Further breaking and weakening of biofilms is achieved using Physical treatment such as ultrasound, laser or photodynamic therapy. While these strategies are promising, they are still hindered by the complexity of biofilm, delivery of treatment and potential resistance. Thus, the use of a multi-modal strategy, targeting different stages of biofilm development, is thought to be the most effective. Finally, a combination of biological, chemical and physical methods provides a promising and effective approach to combat the MDR bacterial infection and enhance the treatment efficacy in the future.

Assessment of Awareness, Attitudes and Practices regarding Antibiotic- Self Medication among University Students.

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Antibiotic self-medication has become a major global public health challenge and is considered one of the leading contributors to antimicrobial resistance (AMR). University students represent a particularly vulnerable population due to increased access to over-the-counter antibiotics, academic stress, previous treatment experiences, limited finances and limited awareness regarding rational antibiotic use. Recent studies conducted in Pakistan and other developing countries report a high prevalence of self-medication practices among students, showing the urgent need for behavioral and educational interventions. The present study aims to assess the awareness, attitudes, and practices regarding antibiotic self-medication among university students through a cross-sectional survey-based approach. A structured and validated questionnaire consisting of demographic, awareness, practice and attitude-related items will be distributed among undergraduate students from different academic disciplines. The attitude section will employ a five-point likerd scale to quantitatively evaluate perceptions and behavioral tendencies related to antibiotic use. Data is analyzed using SPSS software to determine frequencies, mean scores, associations, and correlations between awareness levels and self-medication practices. This study is expected to reveal significant gaps in students' understanding of antibiotic resistance and identify common unsafe practices such as incomplete antibiotic courses, antibiotics use without doctor's prescription, and reliance on pharmacy-based recommendations. The findings will contribute to the growing body of evidence emphasizing the role of educational institutions in combating AMR through awareness campaigns and policy implementation. By integrating public health concerns with microbiological and behavioral perspectives, this research provides valuable insight into antibiotic misuse among young adults and supports global efforts toward responsible antibiotic use and sustainable infection control strategies.

CRISPR-Engineered Bacteriophages as a Novel Therapeutic Strategy against *Escherichia coli* Causing Urinary Tract Infections

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Antimicrobial resistance has emerged as one of the most critical global healthcare threats of the 21st century, with urinary tract infections (UTIs) caused by multidrug-resistant *Escherichia coli* posing a major clinical and economic burden worldwide. The declining efficacy of conventional antibiotics highlights the urgent need for innovative, precision-based antimicrobial therapies. This study proposes the use of CRISPR-engineered bacteriophages as a next-generation therapeutic strategy to specifically target and eradicate resistant *E. coli* strains associated with recurrent UTIs. By integrating the natural bacterial specificity of bacteriophages with the gene-editing power of CRISPR-Cas systems, this approach offers a highly selective and programmable platform capable of disrupting resistance genes while preserving the normal microbiota. The proposed research focuses on the isolation and molecular characterization of uropathogenic *E. coli*, engineering of therapeutic phages, and evaluation of their antibacterial and antibiofilm efficacy. Beyond therapeutic potential, this study explores the future direction of personalized phage medicine, smart antimicrobial delivery systems, and AI-assisted phage design for combating resistant infections. However, challenges including phage-host specificity, regulatory approval, biosafety concerns, immune responses, and large-scale clinical implementation remain important considerations for translational success. Overall, CRISPR-phage therapy represents a revolutionary frontier in biotechnology and precision medicine, offering promising alternatives to traditional antibiotics in the global fight against antimicrobial Resistance.

Use of Stem Cells and CRISPR-Case in Schizophrenia Research and Therapeutics.

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Schizophrenia is a complex polygenic neuropsychiatric disorder affecting millions of people worldwide, characterized by disturbances in cognition, perception, emotion, and behavior. Despite extensive research, current antipsychotic therapies are still limited by poor response rates, severe side effects, and insufficient management of cognitive impairments. Recent advances in stem cell biology and genome editing technologies have opened new opportunities to study molecular and cellular mechanisms of schizophrenia. This review examines the emerging utility of induced pluripotent stem cells (iPSCs) and CRISPR-based technologies in schizophrenia research and therapeutic development. Human iPSC-derived neural models provide a patient-specific platform for studying neuronal dysfunction, synaptic abnormalities, altered signaling pathways, and neural progenitor cell defects in schizophrenia. Moreover, CRISPR/Cas9 allows for precise manipulation of schizophrenia-associated genetic variants, functional genomics studies, and validation of disease-associated loci. The combination of CRISPR and iPSC technology has greatly improved disease modelling by allowing the generation of isogenic controls and the targeted correction of mutations.

Furthermore, multiplexed CRISPR screening approaches have enabled the identification of essential genes involved in neural differentiation and disease pathology. The review also discusses the translational potential of these technologies in personalized medicine, drug discovery, and regenerative therapy, and addresses current technical, ethical, and clinical limitations. In conclusion, stem cell and CRISPR-based strategies are promising tools to promote the knowledge of schizophrenia. They may lead to the development of more effective and personalized therapeutic approaches in the future.

Keywords: Schizophrenia, CRISPR/Cas9, induced pluripotent stem cells, iPSCs, stem cell therapy, genome editing, neuropsychiatric disorders, personalized medicine.

DFT-Guided Next-Generation Na-Ion Batteries Powered by Halogen-Tuned C-12 Nano rings

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Recent research on the design and synthesis of new and upgraded materials for secondary batteries is growing to fulfill future energy demands around the globe. Herein, by using DFT calculations, the thermodynamic and electrochemical properties of Na/Na⁺ @C 12 complexes and then halogens (X⁻ = Br⁻, Cl⁻, and F⁻) as counter anions are studied for the enhancement of Na-ion battery cell voltage and overall performance. Isolated C 12 Nano rings showed a lower cell voltage (−1.32 V), which was significantly increased after adsorption with halide anions as counter anions. Adsorption of halides increased the Gibbs free energy, which in turn resulted in higher cell voltage. Cell voltage increased with the increasing electronegativity of the halide anion. The Gibbs free energy of Br⁻ @C 12 was −52.36 kcal.mol^{−1}, corresponding to a desirable cell voltage of 2.27 V, making it suitable for use as an anode in sodium-ion batteries. The estimated cell voltage of these considered complexes ensures the effective use of these complexes in sodium-ion secondary batteries.

Design and Synthesis of Polyaniline Encapsulated Sulfur Impregnated Porous Carbon Composites as Cathode Material for Advanced Lithium Sulphur Batteries

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Lithium-ion batteries (LiIBs) are struggling to keep pace with advancements in consumer electronics and there are growing need for alternative rechargeable batteries with significantly improved performance. Lithium–sulfur batteries (LiSBs) stand out as one of the most promising beyond LiIBs technologies in terms of both cost and energy density. The synthesized cathode comprises sulfurized polyaniline coated phosphorous doped porous carbon (PANI@S/P-PC) composite. The prepared cathode composites were characterized by Scanning electron microscopy (SEM), Thermal Gravimetric Analysis (TGA), Energy dispersive X-ray (EDX), X-ray diffraction (XRD), Surface Area Analysis (SAA) and Fourier-transform infrared spectroscopy (FTIR) techniques. The composites capacity retention, cyclic performance and rate performance were also investigated. The PANI@S/P-PC composites that were synthesized demonstrated a suitable surface morphology and a high specific surface area of $278 \text{ m}^2 \text{ g}^{-1}$. In lithium-sulfur batteries (Li-SBs), as cathode material, the composites provided an initial capacity of 876 mAh g^{-1} at a current rate of 0.2 C . The capacity showed a low-capacity fading rate of 0.4% per cycle after 100 cycles, staying at 552.2 mAh g^{-1} . Keywords: Energy storage; Cathode materials; Li-Sulfur batteries; Conductive polymer, Composites.

Materials for Dispersive Micro Solid-Phase Extraction: Recent Advances and Analytical Applications

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Dispersive micro solid-phase extraction (D- μ SPE) has emerged as an efficient sample preparation technique due to its simplicity, low solvent consumption, rapid extraction kinetics, and high enrichment factors. Its performance largely depends on the nature of the sorbent material. Recent research has focused on the development of novel extraction materials with enhanced selectivity, extraction efficiency, and reusability for the extraction of trace-level analytes in complex matrices. This presentation reviews the diverse range of materials utilized in D- μ SPE, including carbon-based nanomaterials, magnetic materials, metal-organic frameworks, covalent organic frameworks, molecularly imprinted polymers, ionic liquid-based sorbents, and others. The physicochemical properties of these materials, such as surface area, pore structure, functional groups, and magnetic behavior are critical in determining their extraction efficiency and analytical performance. Applications of these materials in environmental, food, pharmaceutical, and biological analyses are discussed. The advantages, limitations, and future prospects of emerging sorbent materials are also critically discussed.

Photocatalysis: Harnessing Light for Sustainable Chemical Transformations

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Photocatalysis is a sustainable and environmentally friendly technology that utilizes light energy to drive chemical reactions through semiconductor materials. Unlike conventional catalytic processes that often require high temperatures, pressures, or harmful chemicals, photocatalysis operates under mild conditions using solar or artificial light. This technology has attracted significant scientific interest because of its potential applications in environmental remediation, renewable energy production, and green chemical synthesis. Among various semiconductor photocatalysts, zinc oxide (ZnO) has emerged as one of the most widely studied materials due to its low cost, non-toxicity, high chemical stability, and favorable electronic properties. The photocatalytic mechanism begins when ZnO absorbs photons with energy equal to or greater than its band-gap energy. This excitation promotes electrons from the valence band to the conduction band, generating electron–hole pairs. The photogenerated electrons react with oxygen molecules to form superoxide radicals ($\bullet\text{O}_2^-$), while the holes react with water molecules or hydroxide ions to produce hydroxyl radicals ($\bullet\text{OH}$). These highly reactive oxygen species are responsible for degrading organic pollutants, inactivating microorganisms, and facilitating various oxidation–reduction reactions. However, the rapid recombination of electron–hole pairs remains a major challenge that limits photocatalytic efficiency. Recent experimental studies have focused on enhancing ZnO performance through nanostructure engineering, metal and non-metal doping, defect modification, and heterojunction formation. Integration of ZnO with advanced materials such as graphene oxide, reduced graphene oxide, MXenes, and graphitic carbon nitride (g-C₃N₄) has significantly improved visible-light absorption and charge separation efficiency. Furthermore, ZnO nanostructures including nanoparticles, nanorods, nanosheets, and hierarchical composites have demonstrated enhanced photocatalytic activity due to their larger surface area and improved charge transport characteristics. Currently, ZnO-based photocatalysts are extensively investigated for wastewater treatment, degradation of dyes and pharmaceutical contaminants, air purification, antimicrobial coatings, self-cleaning surfaces, photocatalytic hydrogen production, and carbon

dioxide reduction. Continued advances in material design and nanotechnology are expected to improve the efficiency, stability, and scalability of ZnO photocatalysts, making photocatalysis a key technology for sustainable environmental protection and renewable energy generation.

Reconstruction of MOF Material into a Bifunctional Catalytic Water Splitting

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MOFs are reorganized to undergo electrocatalytic polarization, yet the structural evolution of 3D pillared layer MOFs is not well established. A pillared layer CoMOF was investigated to follow the mixed linker environment reconstruction under repeated electrocatalytic activity. The electrochemical activity gradually strips the bipyridine pillars, while parts of the carboxylic linker remain anchored with the metal centers, accompanied by the emergence of thin, sheet-like matrix hosting metal-oxygen. HRTEM reveals lattice-fringe alteration and TEM-EDS analysis show pronounced cobalt-rich composition and suppression of nitrogen content. XPS substantiates mixed metallic(II/III) states and low-binding-energy oxygen steady with the reconstruction. The reconstructed electrocatalyst exhibited outstanding OER activity in the alkaline media, achieving a low overpotential and small Tafel slope, retaining stability over prolonged operation. Additionally, it exhibited remarkable HER activity in both alkaline and acidic media, with exceptionally low η_{10} values and Tafel slopes. The results illustrated a linker-selective reconstruction pathway that transforms a well-defined 3D MOF precursor into an active and robust bifunctional electrocatalyst.

Keywords: MOF; Co MOF; functional electro catalyst; Oxygen evolution; Hydrogen evolution.

Cu-Based MOF-Enhanced Polysulfone Membranes: A Practical Approach to Carbon Capture from Post-Combustion Emissions

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Carbon dioxide (CO₂) is a major contributor to global warming, with its atmospheric concentration continuously rising due to human activities such as fossil fuel combustion, transportation, and industrial processes. One effective approach to tackling this issue is Carbon Capture and Storage (CCS). To advance this strategy, researchers developed high-performance Mixed-Matrix Membranes (MMMs) by incorporating nanocrystals of a newly synthesized Cu (II)-DDA MOF into a polysulfone (PSF) polymer at varying concentrations, using a solution casting technique. The resulting membranes exhibited excellent polymer-filler adhesion, uniform nanoparticle distribution, and strong thermal stability. Gas permeation tests under dry conditions confirmed significant improvements in both CO₂ permeability and CO₂/N₂ selectivity. The optimal formulation containing 10 wt% Cu (II)-DDA MOF, achieved a CO₂ permeability of 15 Barrer and a CO₂/N₂ selectivity of 47, outperforming plain PSF membranes. Notably, these MMMs also maintained their structural integrity and separation efficiency over time, making them a promising and reliable solution for practical carbon capture applications.

Key Words: CO₂ Capture, MMMs, MOF, Polysulfone, Permeability, Selectivity

Designing Green Textile Finishes with Waterborne Polyurethane Dispersions: A Chemistry Driven Approach to Sustainability and Circularity

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Green textile finishes have emerged as a key innovation domain for reconciling highperformance textile functionality with environmental sustainability and circularfashion principles. Recent progress in ecofriendly finishing technologies has focused on replacing conventional, hazardous chemicals with biobased, greensynthesized materials that preserve or even enhance critical properties such as antimicrobial activity, water repellency, UV protection, and flame retardancy. Particular emphasis is placed on how these green finishes support circularity by extending product lifetime, enabling safer endoflife disposal, and improving compatibility with recycling or upcycling routes. By integrating green chemistry, nanotechnology, and sustainable materials design, such approaches offer a pathway to shift textile systems from linear production models toward genuinely sustainable and circular frameworks. In this study, waterborne polyurethane dispersions (FCHB-WPUDs) were synthesized using biobased monomers, such as polyol from fenugreek oil, emulsifier from corn oil. The FCHB-WPUDs, prepared through the prepolymer polymerization route, were characterized using FTIR, TGA, DMA, SEM, DLS, and swelling tests. When applied to poly-cotton fabrics, they significantly enhanced various fabric properties. Notable improvements included washing fastness (3 ± 0.01 to $4/5 \pm 0.03$ for dyed and 3 ± 0.02 to $4/5 \pm 0.02$ for printed fabrics), rubbing fastness ($3/4 \pm 0.02$ to $4/5 \pm 0.02$ for dry dyed and $2/3 \pm 0.02$ to $3/4 \pm 0.03$ for dry printed fabrics), and perspiration fastness ($3/4 \pm 0.01$ to $4/5 \pm 0.02$ for acidic dyed and $3/4 \pm 0.03$ to $4/5 \pm 0.02$ for alkaline printed fabrics). The study offered a more economical and efficient solution for textile finishing.

Keywords: Corn-Fenugreek oil; waterborne polyurethane; physicochemical properties; finishing performance.

POSTER PRESENTATION

A Comparative Study of Transition Metal Oxides and Carbon-Based Metal Materials as dopant in Photocatalytic Water Splitting: Efficiency, Stability, and Mechanistic New Insight.

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The need of clean and sustainable energy in the world has put more pressure on photocatalytic water splitting research as a potential hydrogen production pathway. The speed of such a process depends greatly on the physicochemical characteristics of the photo catalyst. In this review paper, the two major categories of photocatalytic materials Transition Metal Oxides (TMOs) and Carbon-Based Metal Materials (including metal-doped carbon structures, metal-organic frameworks, and carbon-supported metal nanoparticles) have been comparatively analyzed in detail. We assess the performance of TMOs- such as TiO_2 , ZnO , and Fe_2O_3 - historically the most common due to high stability, non-toxicity and cost-effectiveness, but with convenient bandgaps and fast electron-hole recombination. In contrast, we look at metal composites, which are carbon based; graphene-supported metals and graphitic carbon nitride hybrids have great electrical conductivity and have expanded visible-light absorption and large surface areas that increase charge carrier separation. This review will compare the rates of hydrogen evolution (HER), quantum efficiencies and stability lifetimes of both classes of materials by synthesizing the results of the prior studies. The discussion shows that TMOs continue to be the standard of structural strength, but carbon-based metal materials typically have better photocatalytic activity in the visible light because of tuned band structures and efficient interfacial transfer of charge. Nevertheless, in carbon-based systems, there are long-term problems with stability. The review finds that hybrid systems involving the combination of stability of TMOs with the conductivity of carbon supports are the most promising direction of scalable solar hydrogen production so far.

Green Synthesis of Substituted Pyrazolines in Deep Eutectic Solvent and DFT Studies

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Toxic chemicals and volatile organic solvents are major contributors to air pollution, posing serious risks to living organisms. This underscores the need for responsible chemical use and environmentally benign alternatives that minimize harmful effects. Deep eutectic solvents (DES) have emerged as eco-friendly alternative, being cost-effective, less volatile, and biodegradable. In this study, substituted pyrazoline derivatives were synthesized using neutral deep eutectic solvents (NDES) through the reaction of diketones, acetophenones, and hydrazine. The reactions provided excellent yields in shorter reaction times, contributing to sustainable practices that support clean production, environmental protection, and human well-being. The synthesized compounds were thoroughly characterized using Fourier-transform infrared (FTIR) spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, and density functional theory (DFT) calculations. This approach offers an efficient and sustainable route to access pyrazoline derivatives using green solvents.

Keywords: Eco-friendly solvents, deep eutectic solvent, Pyrazine, density functional theory (DFT)

Qualitative and Quantitative Assessment of Sodium Benzoate and Potassium Sorbate preservative in Commercial Beverages by HPLC

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Preservatives are widely used in beverages to prevent spoilage and extend shelf life. In this study, High- Performance Liquid Chromatography (HPLC) was employed to quantify sodium benzoate and potassium sorbate in 30 commercially available soft drink and fruit juice samples. The results revealed notable discrepancies between product labelling and actual preservative content. Sodium benzoate was declared but not detected in ALITA Mango and Quice Apple, while potassium sorbate was detected ($R_t = 1.77$ min) in Pepsi, Coca-Cola, and Fanta despite not being listed on labels. Potassium sorbate concentrations ($0.50\text{--}1.26\text{ }\mu\text{g/mL}$) complied with European Food Safety Authority (EFSA) limits. In contrast, sodium benzoate levels in beverages such as Sting Gold Rush, Coca-Cola, Gourmet Cola, and Pepsi exceeded the EFSA limit of $5\text{ }\mu\text{g/mL}$, reaching up to $25.83\text{ }\mu\text{g/mL}$ ($R_t = 1.88$ min). These findings underscore the need for stricter regulatory monitoring and accurate labelling to ensure consumer safety.

Keywords: High-Performance Liquid Chromatography (HPLC), Sodium Benzoate, Potassium Sorbate, Food Preservatives.

Synthesis and Characterization of Biochar/BaTiO₃ Composite for Adsorptive Removal of Industrial Dyes

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The presence of industrial effluents that have synthetic dyes constitutes an important environmental issue due to its toxicity, stability and resistance to degradation. As presented in this publication, an adsorbent was prepared using biochar barium titanate (BaTiO₃) in the process of removing industrial dyes in aqueous media. Biochar was produced from *Citrullus colocynthis* via pyrolysis under oxygen-limited conditions, yielding a porous carbonaceous material enriched with diverse surface functional groups. At the same time, the well-known piezoelectric ceramic was prepared using the solid-state reaction approach with starting materials being BaCO₃ and TiO₂ that were then combined with biochar to make the composite; this was called BaTiO₃. Isotherm models were used to assess equilibrium adsorption behavior, and the composite was found to have a maximum adsorption capacity ($q_{\max}$) of 6.43 mg/g, albeit with no doubt that the composite can be used with dyes. The biochar skeleton provided a large quantity of active adsorption sites, and BaTiO₃ provided functional properties that could enhance interfacial interactions in the composite system.

The proposed research contributes to the sustainable design of materials by converting biomass waste into biochar, which has a value, which in turn promotes sustainable development goal 12 (Responsible Consumption and Production). Further, the biochar ability to sequester carbon conforms to Sustainable Development Goal 13 (Climate Action). In general, the suggested composite offers an ecological-friendly and sustainable approach to the treatment of dye-contaminated industrial wastewater.

Zn–Cu BDC Bimetallic MOFs as Efficient Bifunctional Electrocatalysts for Sustainable Water Splitting and Hydrogen Production

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The research work outlined the catalytic behavior of transition metals like Zn and Cu metallic centers in Zn-Cu BDC BMOFs utilized for sustainable hydrogen production. Zn-Cu BDC bimetallic MOF fabricated through one-pot solvothermal of multifunctional metallic precursors with organic linker 1:1 molar ratio. Crystalline BMOFs incorporated on surface of Nickle foam which further utilize to study electrochemical parameters LSV, CV and EIS in 1M KOH solution. BMOFs clarify limitations through heterometallic active sites which enhanced the electrochemical activity during HER and OER processes. Zn-Cu BMOFs exhibit outstanding bifunctional performance in 1M KOH, indicating overpotential of 248mV (OER) and 178mV (HER) at 10mA cm⁻² with Tafel slopes of 70mV dec⁻¹ at OER and 84mV dec⁻¹ at HER. ECSA value was estimated 32.5 cm² indicates significant number of active sites are available. Double-layer capacitance (Cdl) for the catalyst was about 1.30mF cm⁻² indicate moderate electrochemically active surface area for electrocatalytic process. EIS curve indicates reduce charge-transfer resistance []. Impedance data point out small Rs value approximately 0.93Ω led to favorable ionic conductivity and better electrocatalytic reaction. Study highlights the synthetic and structural based framework for advance Zn-Cu BDC MOFs as an earth abundant bifunctional, and sustainable electrocatalyst. Characterization utilizes i.e. SEM, FTIR, and XRD for the effective preparation of the bimetallic MOFs. BMOFs were recognized with their high porosity and thermal stability and firm structure of the metals with organic ligands. MOFs have been characterized by using various techniques (SEM) investigated morphology (shape and size), XRD measured phase structure, FTIR studied chemical properties of MOFs. In future more Investigation requires for the long-term stability and recyclability of Zn-Cu BDC MOFs in real-world applications.

Comparative Analysis of Antispasmodic Activity of the Genus *Mentha*

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Essential oils derived from aromatic plants are recognized for their medicinal, preventive, and economic significance. Among medicinal plants, mint (*Mentha* species) exhibits multiple health-beneficial properties. The extracts and essential oils derived from the genus *Mentha* are commonly used in folk medicine. It is most widely used to treat respiratory issues as an expectorant and anti-congestant, and as an antispasmodic for the digestive and vascular systems.

In this study, six reported methodologies were compared to evaluate the antispasmodic activity of various *Mentha* species, including *Mentha piperita*, *Mentha pulegium*, *Mentha longifolia*, *Mentha suaveolens* Ehrh, and extracts/essential oils to determine which approach demonstrated the strongest relaxant potential. Different parameters, including the dose range, IC₅₀ values, and

% relaxation, were compared to determine the most efficient method and *Mentha* extract/essential oil for the relaxation effects. Among them, the essential oil of *Mentha pulegium* L., with a 1-300 µg/mL dose range, on the trachea and bladder strips of the Male Wistar rat, demonstrated the strongest antispasmodic activity. The analysis of the mechanism of action of *M. pulegium* suggested that the antispasmodic effects were observed due to K⁺ and ACh-induced relaxation. It exhibited an IC₅₀ value of 0.04047 mg/mL, with a maximum percentage relaxation of 120%. The comparative analysis suggests that *M. pulegium* has greater relaxant potential on smooth muscle than the extracts of *M. piperita*, *M. suaveolens*, and *M. longifolia*.

Comparative Study of Green Synthesis of Zinc Oxide Nano-Particles

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In the present study, a comparative investigation was conducted on The nano-scale zinc oxide (ZnO NPs) was synthesized using leaf extract by an eco-friendly method extracts of *Vernonia cinerea* and *Aloe barbadensis* Mill. As biogenic reducing, stabilizing, and capping agents. The phytogenic ZnO NPs were specified using UV–Visible spectroscopy, FTIR, X-ray diffraction (XRD), energy-dispersive X-ray (EDX), and field emission scanning electron microscopy (FESEM), confirming their crystalline nature, high purity, spherical morphology, and nano-size range (~35 nm). In comparison to chemically synthesized ZnO NPs (~48 nm) the green ZnO NPs exhibited superior properties attributed to the high reducing property of the plant extracts. The bio-synthesized ZnO The potential of the NPs was analyzed. Role in promoting plant growth and mitigating heavy metal stress. In tomato (*Solanum lycopersicum* L.) and wheat (*Triticum aestivum* L.) seedlings, ZnO NPs at lower concentrations significantly enhanced seed germination, shoot and root elongation, and overall seedling vigor. In tomato plants, ZnO NPs also improved physiological and morphological traits, including stem width, leaf density, plant-based richness, and fruit yield. Among six treatment concentrations, 99.076 ppm ZnO NPs yielded the most significant improvements across measured growth parameters. Moreover, in Pb-stressed tomato seedlings, ZnO NPs at 50 mg/L mitigated oxidative stress by enhancing chlorophyll content, protein levels, sugar constituents, nitrate reductase activity, and the activity of crucial antioxidant enzymes such as superoxide dismutase, catalase, and ascorbate peroxidase. These findings underscore the dual functionality of green ZnO NPs as both a biofertilizer and stress alleviator. In conclusion, biogenically synthesized ZnO NPs Statistically significant improvement ($p < 0.05$) was observed in growth and antioxidant parameters at optimized concentration not only promote growth and productivity in economically important crops like tomato and wheat but also offer potential as a nano-nutrient and bioprotective agent against environmental stressors such as heavy metals, paving the way for sustainable agricultural practices.

Phytochemical Composition, Antioxidant, and Antimicrobial Activities of *Abutilon indicum* (L.) Sweet: A Comparative Review

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Abutilon indicum (L.) Sweet (Malvaceae) is a widely used medicinal plant whose phytochemical profile helps explain its antioxidant and antimicrobial effects. Evidence across plant parts indicates that phenolics, flavonoids, saponins, and unsaturated fatty acids are the dominant bioactive constituents. Analyses of seed oil show a high proportion of unsaturated fatty acids, particularly linoleic and oleic acids, together with high phenolic content and broad- spectrum antibacterial activity. An alcoholic extract that included a chloroform fraction demonstrated strong DPPH radical scavenging activity (87.6%) and showed notable antibacterial and antifungal effects. Methanolic leaf extracts increased ferric reducing antioxidant power (FRAP) in a concentration-dependent manner, confirming meaningful reducing capacity. Leaf saponin extracts also showed very high antioxidant performance (96.17% DPPH inhibition) and effective antibacterial activity, with reports indicating no associated DNA damage. More recently, in-vitro callus cultures were reported to contain higher phenolic content (10.56 µg/mL) and the greatest antioxidant potential among examined tissues, suggesting that tissue culture can enhance the production of bioactive compounds. Overall, the literature supports *A. indicum* as a valuable source of phenolics and flavonoids that underpin its antioxidant, antibacterial, and antifungal actions, encouraging its development for pharmaceutical, nutraceutical, and cosmetic applications. Across studies, antioxidant capacity was commonly assessed using DPPH and FRAP assays; activity remained high across solvents, although extract polarity often altered yields. Antimicrobial reports included both bacteria and fungi. Overall, choosing suitable plant parts, extraction conditions, and callus culture strategies may help optimize bioactive recovery for practical formulations. These steps also support evidence-based standardization for future product development.

Comparative Analysis of Vitamin C, Polyphenols, and Antioxidant Activity in Wild and Cultivated Crab Apples

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This comparison reports the phytochemical profile, vitamin C levels, and antioxidant activity of the *Malus* genus, encompassing crab apples and wild apples. Studies showed that the fruits of *Malus sylvestris* have a new, stable vitamin C glycoside (2-O- β -D-glucopyranosyl-L-ascorbic acid) that is very resistant to oxidation and has strong antioxidant properties. Research on *Malus baccata* shows that it contains a variety of phenolic and flavonoid compounds. These compounds are pivotal in maintaining human health. *Malus baccata* also has an ability to stop free radicals with DPPH and FRAP. The *Malus* ‘Royalty’ had the effect on stopping these free radicals. This was seen when it was compared to crab apple types like *Malus* ‘Pink Perfection’ and *Malus zumi* ‘Golden Hornet’. *Malus* ‘Royalty’ was the best, at this. The amount of vitamin C and phenolic compounds is different in the three varieties of apples. It goes from 1.2 to 5.9 mg of vitamin C and phenolic compounds per 100 grams of apples. While observing that the press cakes and other things which are left over from apples, we can see that they have a lot of vitamin C and phenolic compounds. In fact, they have as much as 6.8 grams of phenolic compounds and 564 milligrams of vitamin C per 100 grams of these wild apple by-products. This makes vitamin C and phenolic compounds from apples a great source of good health, and environment friendly. These findings collectively confirming that *Malus* species and their processing by-products can be used as significant natural sources of phenolics, flavonoids, and vitamin C derivatives, showing robust antioxidant properties and potential applications in functional foods, nutraceuticals, and natural antioxidant formulations.

Diversity in Antioxidant Properties of the Genus *Dioscorea*: A Comparative Study of Five Species

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The genus *Dioscorea* is a taxonomically heterogeneous group of tuberous plants that represents a crucial cross bound between nutritional security in the world and the investigation of natural bioactivity potential. This study focuses on the biochemical composition of five different species namely as *D.wallichii*, *D.hispida*, *D.tomentosa*, *D.alata* and *D.bulbifera* to explain their unique phytochemical compositions as well as to comparatively analyse their anti-oxidant activity. Quantitative analysis of these species reveals that there are high concentrations of total phenolics and flavonoids that are present in methanolic fractions which are major facilitators of the electron donations and hydrogen atom transfer processes. A considerable finding is the multifunctional bioactivity demonstrated by these species which effectively encompasses potent antioxidant activity in conjunction with therapeutic activity for membrane stabilization against hypotonicity induced haemolysis and thrombolysis via clot lysis. Furthermore, the specialized metabolites like anthocyanins, tannins and steroidal saponins like diosgenin are responsible for strong antiproliferative properties and inhibition of nitric oxide and superoxide radicals. A strong positive correlation is found between total phenolic content (TPC) and ferric reducing antioxidant power (FRAP) suggest that these species are significant reservoirs of natural reductones. The comparative synthesis concludes that *Dioscorea* genus possess a unique signature of metabolism that can neutralize various reactive oxygen species (ROS) and inhibiting oxidative damage. *D.wallichii* and *D.hispida* tend to show better potency and wide range of pharmacological activities. These findings validate the pharmacological claims associated with the wild and cultivated varieties suggesting significant scope for the incorporation of these species into high value functional foods and pharmaceutical agents targeting oxidative stress related pathogens and other metabolic disorders.

Sustainable Remediation of Diamond Green G Laden- Wastewater via Oxalic-Acid Modified Amerimnon Sissoo Sawmill Waste

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This study looks into the remediation of Diamond Green G from a mixture of industrial effluents in an efficacious way by utilizing a designed bio sorbent composed of an Amerimnon sissoo wood waste. Microwave-assisted oxalic acid functionalization was used to transform raw biomass into the better adsorbent with maximum monolayer capacity of 9.69 mg/g, almost twice the capacity of the precursor material. SEM, EDX and FTIR surface analysis proved the successful development of active binding sites as a result of treatment and optimal morphology.

The batch experiments revealed that the sequestration reaction follows pseudo-second order kinetics ($R^2 = 1$) and the Freundlich isotherm, which implies that there is strong multi-layer adsorption on a heterogeneous surface and maximum removal was observed when pH of the effluent was acidic. It was discovered that the process was spontaneous and exothermic and it gave a high removal rate of 93.04% when tested in real industrial effluents in just 30mins. These results underline how industrial wastewater is treated, with the emphasis on waste repurposing and the environmental sustainability, which is scalable and energy-saving. Consistent performance over seven regeneration cycles, ease of operation and secure end-of-life disposal procedure are some of the reasons why this study offers a low-energy, circular economy wastewater detoxification solution at Industrial scale.

Keywords: Adsorption, Diamond Green G, Amerimnon sissoo, Regeneration, isotherm and kinetics, Thermodynamic studies, bio sorption, oxalic acid, Industrial wastewater remediation, Circular economy, Environmental sustainability.

***In Silico* Discovery of HPV 16 Inhibitors by Molecular Docking, Molecular Simulations and DFT Studies**

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Human papillomavirus type 16 is a high-risk oncogenic genotype and is strongly associated with cervical cancer and other malignancies. Although the development of prophylactic vaccines has greatly reduced the prevalence of HPV infections, these vaccines are not effective in eliminating pre-existing infections and highlight the need to develop effective inhibitors of HPV16-derived targets. In the present investigation, an in-silico approach based on molecular docking and molecular dynamics simulations was used to assess the inhibitory potential of the selected compounds With anolide E, SCHEMBL26679511, and MLS000728579 against the selected target protein of HPV16. The best docking poses of the compounds were used for 100 ns MD simulations to assess their stability and flexibility in terms of structural stability, conformational adaptation, and residue flexibility, compactness of the protein-ligand complex, solvent accessibility, intermolecular interactions, and binding affinity. The MD simulation revealed different patterns of dynamic behavior of the protein-ligand complexes of the three compounds. The With anolide E-HPV16 complex showed relatively higher values of backbone and ligand RMSD values, indicating significant conformational adaptation during the MD simulation period; however, stable values of minimum distance and intermolecular interactions indicated persistent binding of the ligand to the protein target. The SCHEMBL26679511-HPV16 complex showed moderate values of backbone RMSD and relatively low values of ligand RMSD, indicating good positional stability of the ligand within the active site of the protein; however, low values of hydrogen bond occupancy and structural variations in the later stages of the simulation period were noted. In contrast to these complexes, the MLS000728579-HPV16 complex showed the best dynamic behavior in terms of stable values of backbone RMSD, constant values of radius of gyration, stable values of solvent accessibility, persistent values of hydrogen bond interactions, and persistent values of protein-ligand interactions during the entire period of the MD simulation. Furthermore, the RMSF values indicated that the protein showed maximum flexibility at the terminal and loop regions; however,

the core region of the protein showed stable structural behavior. The results of the present investigation revealed that all the compounds showed good binding affinity to the selected target protein of HPV16; however, the MLS000728579-HPV16 complex showed the best dynamic behavior followed by SCHEMBL26679511 and with anolide E-HPV16 complexes.

Comparative Analysis of Silicon Based Anode in Lithium-Ion Batteries (Secondary Batteries)

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The increased need for lithium-ion batteries (LIBs) that offer greater energy density has intensified research for alternatives to typical greenhouse anodes, leading to promising research for silicon-based anode materials. Silicon has an incredibly high theoretical capacity of 4200 mAh g^{-1} , which greatly surpasses what commercial graphite anodes can provide. This is also the case for lithium storage capacity for silicon oxides like SiO_2 and SiO_x . Despite the advantages, practical use is not achievable. Silicon has an enormous volume expansion of three times its original volume during lithiation leading to a multitude of problems including rapid capacity fading during charge-discharge cycles, stress related fractures, unstable solid electrolyte interphase (SEI) formations, and rapid increases in electrical resistance. Recent research has focused on the structural design and composite engineering of silicon. Silicon-carbon composites are more electrochemically stable than normal silicon anodes and also enhance electrical conductivity by active mass buffering and volume expansion. The collapsing mesoporous silica framework and surface functionalization with metal oxides like TiO_2 , and GeO_2 also increased overall structural integrity along with columbic efficiency masking a significant amount of volume expansion. The SiO_x/C composites and their oxide scaffold help to maintain mechanical stability while alleviate the volume expansion. Additionally, performance of the composite has also been supplemented by doping, while n type doping has also shown. According to Texas Instruments, N-type doping has benefits for rate capability and cycling stability while some P-type dopants are known to speed up capacity loss. Furthermore, the improved lithium diffusion kinetics and structural/ mechanical stability of amorphous Si, make it superior to C-Si. Scalable fabrication techniques, like the embedding of Si in graphitized carbon xerogels and the inclusion of graphitic oxides, result in composite anodes with improved cycling stability and reversible capacity >90% of original capacity remained after extensive cycling due to advanced nano structuring of SiO_2 nanoparticles encapsulated in carbon nanosheets. Hybrid SiO_x ($x \sim 0$), amorphous carbon, and few-layer graphene (FLG)

nanocomposites showed excellent full cell performance. Overall, continuous improvement of material design and nano structuring along with compositional optimization are important to minimize the remaining obstacles to large-scale, fully industrialized silicon-based battery anodes for LIBs.

Comparative Analysis of Titanium Dioxide Nanoparticles in Sunscreens: Evaluation of Morphology, Penetration, and Safety

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Titanium dioxide nanoparticles (TiO₂ NPs) are commonly utilized in sunscreen products because of their superior ultraviolet (UV) blocking capability and optical clarity. Nonetheless, worries about their safety, such as skin penetration and the potential to cause oxidative stress, continue to be a focus of ongoing research. This research seeks to compare the morphology, penetration characteristics, and safety features of TiO₂ nanoparticles utilized in sunscreens. A comparative examination was performed utilizing five recent research studies. Different analytical and characterization methods, such as Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), X-ray Diffraction (XRD), Energy Dispersive Spectroscopy (EDS), and Particle Size Analysis (PSA), were employed to assess nanoparticle morphology, size, and composition. Biological evaluations including MTT cytotoxicity assay, reactive oxygen species (ROS) analysis, along with in vitro and in vivo skin penetration investigations (Franz diffusion cells and human studies) were likewise examined. The findings suggest that the majority of TiO₂ nanoparticles are within the nanoscale spectrum and show significant UV protection properties. Although limited skin penetration was noted in many stances, some research indicated nanoparticle absorption and oxidative stress under particular circumstances. Differences in particle size, shape, surface treatment, and TiO₂ levels markedly affected both effectiveness and safety profiles. To summarize, TiO₂ nanoparticles continue to function as efficient UV filters in sunscreen products; nevertheless, their safety relies on physicochemical characteristics and the design of the formulation. Ongoing assessment and advancement of safer, biocompatible options are vital to guarantee consumer safety and product effectiveness.

Keywords: Biocompatibility, Nano toxicity, Oxidative stress, Skin penetration, Sunscreen formulations, Titanium dioxide nanoparticles, UV protection.

Synthesis and Characterization of Plant Mediated Silver Nanoparticles using turmeric and extracts of *Azadirachta indica* and Green tea

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The green synthesis of silver nanoparticles (AgNPs) has gained much attention due to its eco-friendly, cost-effective and sustainable method. In this research the synthesis and characterization of plant mediated AgNPs using extract of neem, green tea and turmeric as natural reducing and capping agents are studied. The antibacterial and sensor activities of the AgNPs are also investigated. Neem-turmeric and green tea-turmeric extracts were prepared by heating powdered plant materials in distilled water and filtration. The extracts were mixed with silver nitrate solution with continuous stirring and then centrifugation in order to promote the formation of AgNPs. The nanoparticles formation, morphology, crystallinity and surface functional groups were confirmed by UV–Visible spectroscopy, EDX, XRD and SEM analysis. The electroconductive performance was evaluated by the electrochemical properties such as Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS). AgNP synthesis was confirmed by a prominent color change and UV–Visible peaks at 400–450 nm. SEM showed nanoparticles formation shapes, EDX confirmed Silver peaks and XRD confirmed crystallinity. The electrochemical characterization showed that the AgNPs modified electrodes had a higher electron transfer and lower charge transfer resistance than the bare ones, suggesting their excellent potential as sensors. The antibacterial activity against the target strains was evaluated by Zone of inhibition methods. The results show the antibacterial and electrochemical potential of neem-, green tea-, and turmeric-mediated AgNPs, highlighting their importance in green nanotechnology, biomedicine, and electrochemical sensing.

Eco-Friendly Acid Pickling for Industrial Derusting Using Food-Grade Organic Acids and Fruit-Waste Extracts

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Rusting of carbon steels imposes a significant economic burden across industrial infrastructure. Industrial derusting through acid pickling commonly uses mineral acids such as hydrochloric acid and sulfuric acid, which generate toxic fumes, pose corrosive hazards, and require costly disposal. This study investigates eco-friendly pickling alternatives based on food-grade organic acids and fruit-waste extracts to address these concerns. Tartaric acid was used as a chelating agent and progressively combined with ascorbic acid (reducing agent), sodium bicarbonate (pH modulator), ethanol (wetting agent), and aqueous extracts of banana (*Musa acuminata*) and orange (*Citrus sinensis*) peels to produce eight formulations. Pre-rusted mild steel coupons were immersed for 24 h at $28 \pm 2^\circ\text{C}$. Derusting efficiency was quantified gravimetrically, and solutions were characterized by pH and conductivity, while attenuated total reflectance Fourier-transform infrared spectroscopy was used to study dissolution mechanisms. Formulation containing both peel extracts achieved highest efficiency of $90.8 \pm 1.9\%$. Derusting performance was modeled using Gaussian Process. Regression achieving test coefficient of determination of 0.98 (root mean square error = 1.2%). Model-guided refinement increased efficiency to $94.2 \pm 1.5\%$, comparable to $96.7 \pm 1.1\%$ of 10% hydrochloric acid under identical conditions. Spectroscopy confirmed rust dissolution through iron chelation rather than proton-driven substrate attack, with no surface etching observed. This biodegradable formulation derived from food-safe reagents and fruit by-products reduces occupational exposure and disposal costs. These findings demonstrate a viable safer alternative to mineral acid pickling, supporting responsible consumption and production (United Nations Sustainable Development Goal 12) and advancing sustainable corrosion management.

Keywords: acid pickling, mild steel corrosion, organic acids, fruit peel extracts, Gaussian Process Regression

Graphene Oxide-Based Polyethersulfone Membranes for Water Purification

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PES membranes containing different concentrations of GO, PVP, and PEG were prepared by phase immersion. These membranes are widely used in water purification. Characterization by XRD, SEM, and FTIR confirmed improved GO dispersion, hydrophilicity, and porous structure. GO-incorporated membranes showed enhanced water flux ($95 \text{ L} \cdot \text{m}^{-2} \cdot \text{h}^{-1}$), higher salt rejection (72%), better wettability, and improved antibacterial activity against *S. aureus* and *E. coli* compared to pristine PES membranes.

Antifouling and Flux Enhancement of Grafted Reverse Osmosis Membrane by ATRP

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This research focuses on synthesizing Fe doped titanium oxide nanoparticles to overcome UV-only absorption limitation of pure titanium oxide. Using a controlled co - precipitation method with isoamyl alcohol and thermal treatment, the band gap is shifted for visible light activity, while retaining the critical anatase phase (approx.177 nm size). The resulting materials show promise as effective photocatalyst, antibacterial agents and target it drug delivery vehicles.

**Biobased and Biodegradable Polymers, Progress In Chemistry, and
Environmental Implications MoS₂/Hbn Van Der Waals Heterostructures:
Interfacial Chemistry, Protective Coatings, and Emerging Applications**

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Biodegradable and biobased polymers (BBPs) have emerged as sustainable alternatives to conventional plastics due to increasing plastic waste and microplastic pollution. BBPs are derived from renewable feedstocks and undergo microbial degradation under suitable environmental conditions. Recent advancements in polymer modification have improved their mechanical properties and expanded applications in packaging, agriculture, and biomedical fields. BBPs can reduce environmental pollution, protect ecosystems, and support the development of a sustainable circular economy.

MoS₂/hBN Van der Waals Heterostructures: Interfacial Chemistry, Protective Coatings, and Emerging Applications

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MoS₂/hBN heterostructures are advanced two-dimensional (2D) van der Waals materials composed of semiconducting molybdenum disulfide (MoS₂) and electrically insulating hexagonal boron nitride (hBN). This combination integrates the excellent tribological and electronic properties of MoS₂ with the chemical inertness, thermal stability, and dielectric characteristics of hBN. Weak interlayer interactions and atomically smooth interfaces preserve the intrinsic properties of both materials while enabling tunable electronic, optical, and interfacial behavior. MoS₂ is widely used as a solid lubricant due to its low friction and wear resistance; however, its application is limited by oxidation and corrosion under humid conditions. Incorporation of hBN improves environmental stability by suppressing oxidation and enhancing corrosion resistance. The layered MoS₂–hBN structure also reduces porosity and limits the diffusion of corrosive species, improving coating performance and durability. Owing to their unique properties, MoS₂/hBN heterostructures have applications in protective coatings, tribology, nanoelectronics, energy storage, sensors, catalysis, and AI-enabled technologies, making them promising materials for next-generation sustainable and multifunctional Systems.

***In silico* Discovery of Novel Hantavirus Inhibitors from Natural Products: An Integrated Study using DFT, Molecular Docking, and MD Simulations**

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Hantavirus is a dangerous zoonotic virus transmitted mainly through infected rodents and is responsible for severe illnesses such as Hemorrhagic Fever with Renal Syndrome (HFRS) and Hantavirus Cardiopulmonary Syndrome (HCPS). These diseases can become fatal if not treated promptly, and currently there are no approved antiviral drugs or fully effective vaccines available specifically for hantavirus infections. Because of this, identifying new therapeutic agents has become an important area of research. One of the most promising antiviral targets is the viral L protein cap-snatching endonuclease, which plays a key role in viral replication and transcription. In this study, an integrated computational strategy was applied to discover potential natural inhibitors against hantavirus. A total of 212 phytochemical compounds obtained from natural products were evaluated through different *in silico* techniques, including pharmacokinetic screening, molecular docking, Density Functional Theory (DFT) analysis, and Molecular Dynamics (MD) simulations. Drug-likeness analysis using SwissADME confirmed that the shortlisted compounds followed Lipinski's Rule of Five, indicating favorable pharmaceutical properties. Molecular docking studies were carried out on the Hantaan virus L protein endonuclease (PDB ID: 5IZE) using AutoDock Vina. Among all screened compounds, ligand125 demonstrated the strongest interaction with the target protein, showing a binding affinity of -8.838 kcal/mol, while ligand207 also showed promising results with -8.171 kcal/mol. Further electronic structure analysis using DFT at the B3LYP/6-31G(d,p) level revealed that ligand125 possesses high electronic stability and chemical robustness, reflected by its favorable HOMO-LUMO energy gap. RMSD, hydrogen bonding behavior, and solvent-accessible surface area analyses collectively supported the structural stability of the protein-ligand complex. Overall, the findings suggest that ligand125 could serve as a promising natural-product-based inhibitor against hantavirus and may be considered a strong candidate for future experimental and pharmaceutical investigations.

Development of Thermosetting Precursors and Copolymers for High Performance Thermal Protection Epoxy/Phenolic System

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Abstract: This study focuses on the synthesis and utilization of thermosetting precursors, namely boron polyol, benzoxazine monomer, and borate ester for the development of high-performance polymeric thermal protection systems. Boron polyol and borate ester were combined with aerospace-grade epoxy resins to form thermosets/blends. Meanwhile, the benzoxazine monomer was copolymerized with epoxy resin and resole to enhance their thermal properties. The chemical structures of the synthesized precursors were thoroughly characterized using Fourier-transform infrared spectroscopy (FTIR). Flame retardancy performance was evaluated through UL-94 vertical burning test, which demonstrated significant improvements in thermal stability and fire resistance compared to neat epoxy and resole systems. This study highlights the potential of the developed precursors and copolymers as promising candidates for use in high-temperature applications, particularly in the aerospace sectors, where excellent flame retardancy and thermal stability requirements are critical.

Fabrication of Iron Oxide Nanorings Doped with Second-Row Transition Metals for Use as Single-Atom Catalysts in Hydrogen Evolution Reactions

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The hydrogen evolution process (HER) is receiving more attention from scientists as a key component of sustainable energy. The cutting edge of electrocatalysis is represented by single-atom catalysts (SACs), which provide excellent electrical conductivity, strong thermal stability, and maximum atom utilization. The catalytic potential of iron oxide nanorings for HER is assessed in this work using Density Functional Theory (DFT), with all simulations carried out at the ω B97XD/def2-SVP level of theory. This study explores an optimization technique that involves fabricating second-row transition metals (TMs) doped onto the nanoring framework, since virgin iron oxide structures frequently show minimal HER activity. These TMs have the potential to greatly improve catalytic sites and are chosen due to their considerable abundance and affordability in comparison to noble metals. By computing enthalpy, entropy, and Gibbs free energy (ΔG), the study aims to methodically assess the thermodynamic stability of the H-adsorbed systems. The electronic properties, such as Density of States (DOS), Non-Covalent Interaction (NCI) analysis, Natural Bond Orbital (NBO) analysis, and Frontier Molecular Orbitals (FMOs), are being investigated in order to provide a thorough understanding of the catalytic mechanism. Finding a dopant arrangement that minimizes over-potential by achieving a ΔG value close to the ideal 0 eV threshold is the main goal. The purpose of this work is to demonstrate TM-doped iron oxide nanorings, potential as high-efficiency SAC systems for upcoming HER applications.

Synthesis and Characterization of Plant Mediated Silver Nanoparticles using Turmeric and Extracts of *Moringa oleifera* and Black tea

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By using plant extracts as natural reducing and stabilizing agents, green synthesis of silver nanoparticles (AgNPs) is a sustainable, economical, and environmentally friendly method that does away with the need for hazardous chemicals. The important antibacterial, catalytic, and optical qualities of silver nanoparticles are well known. Plant extracts of black tea (*Camellia sinensis*), turmeric (*Curcuma longa*), and *Moringa oleifera* were used in this work to create AgNPs. These extracts are rich in bioactive substances like curcumin, polyphenols, and flavonoids that aid in the production and stability of nanoparticles. Plant materials were heated with distilled water to create plant extracts, which were then filtered to produce clear solutions that included phytochemicals. The reduction of silver ions into silver nanoparticles was first verified by a noticeable color shift when these extracts were individually combined with silver nitrate (AgNO_3) solution while being continuously stirred. UV-visible spectroscopy was used to confirm the production of AgNPs. The antibacterial activity of the produced nanoparticles was then assessed. The outcomes verified that all three plant extracts were successfully used to create silver nanoparticles. *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Staphylococcus gallinarum*, and *Pseudomonas aeruginosa* were the four bacterial strains against which the antibacterial activity was evaluated using the zone of inhibition technique, demonstrating discernible inhibitory effects. In summary, our work shows how to synthesize silver nanoparticles utilizing extracts from medicinal plants in an effective, straightforward, and eco-friendly manner. The biosynthesized AgNPs show encouraging antibacterial properties, demonstrating their suitability for use in environmental and biomedical domains.

AI-Powered Microplastics Monitoring in Water

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The widespread presence of microplastic pollution in aquatic environments and drinking water sources has become a major environmental and public health worry. As micro-plastics have been discovered in both municipal and industrial water supplies, there is a need for effective, reliable and scalable monitoring strategies. Traditional microplastic identification techniques are time consuming, labor intensive, and rely on manual microscope examination. The objective of this study is to build an artificial intelligence-based system for microplastic detection and monitoring in different water bodies. Water samples will be gathered from various water sources such as tap water, filtered water, boiled tap water, boiled filtered water, grey water and other water sources commonly used. The samples collected will be sent for microscopic analysis in order to identify and characterize possible microplastic particles. Microscopy-based image data will be used to assist the development of a system that will use artificial intelligence to more efficiently and consistently recognise and classify microplastic contamination. The study is anticipated to shed light on the occurrence of micro-plastic contamination in various water sources as well as the feasibility of AI image analysis for water monitoring. This study aims to apply artificial intelligence to traditional microscopy to help with faster and more accurate environmental monitoring of micro plastics. The results can contribute to future water quality assessments, pollution control, and sustainable solutions to safeguarding public health and water bodies.

Hetrostructure Ti- doped SnO₂ /gC₃N₄ Nano Composite for Enhance Photocatalytic Degradation of Organic Pollutant and Antibacterial Application

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The increase in environmental pollution and bacterial contamination has highlighted the need of efficient visible light active photo catalyst. In this comparative study Ti-doped SnO₂/gC₃N₄ heterostructure Nano composites shows highly effective photocatalytic and microbial activity. The mutual enhancement of Ti doped SnO₂/gC₃N₄ shows enhanced visible light harvesting, rapid charge carrier migration and reduce electron-hole recombination, results in enhanced photocatalytic activity. The enhanced regeneration of reactive oxygen species results in efficient degradation of organic pollutants and dyes. In addition to this Nano composite shows remarkable antibacterial activity against gram positive and gram negative bacteria via oxidative membrane damage. The enhanced photocatalytic activity was attributed to defect engineering, increased density of catalytic active sites, and optimized heterointerface construction. The study demonstrate Ti-doped SnO₂/g-C₃N₄ heterostructure as a promising multifunctional photo catalysts for waste water remediation and antibacterial applications.

Comparative Scientific Analysis of Onion Peel-Based Anti-Aging Cream Formulations

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This study presents the formulation and comparative evaluation of an *Allium cepa* (onion) peel-based anti-aging cream enriched with bioactive phytochemicals, including quercetin, kaempferol, anthocyanins, and sulfur-containing phenolics. The developed formulation exhibited strong antioxidant potential (~82% DPPH radical scavenging), indicating efficient suppression of oxidative stress-mediated skin aging processes. Enzymatic inhibition assays revealed significant reduction in collagenase and elastase activities, demonstrating effective protection of extracellular matrix components via modulation of MMP-associated pathways. The formulation further showed enhanced dermal hydration (~70% increase) and superior physicochemical stability compared to the control base cream. In addition, notable antimicrobial activity against *Staphylococcus aureus* and *Escherichia coli* confirmed its dermo protective and preservative efficacy. Overall, the synergistic action of flavonoids and phenolic compounds establishes onion peel extract as a sustainable, multi-targeted, and high-potential cosmeceutical agent for advanced anti-aging skincare applications.

Ni/Co-based MIL-88 Layered by Layered Nanomaterial for Aqueous Hybrid Supercapacitors

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Aqueous hybrid supercapacitors are safer and more sustainable than traditional electrochemical energy storage devices that use toxic and pyrophoric organic electrolytes. Metal-organic frameworks (MOFs) have attracted significant interest for energy storage applications because of their large pore size, durability, and charge-storing potential. MOFs, especially MIL-88, exhibit adjustable porosity and abundant redox-active sites. MIL-88 was synthesized by the solvothermal method, and its charge-storing ability was investigated. The successful formation of the MIL-88 framework and the addition of Ni/Co nanoparticles were verified by different analytical techniques. FTIR shows peaks near 1600 cm^{-1} and $1380\text{--}1450\text{ cm}^{-1}$ were identified as the asymmetric and symmetric stretching vibrations of the organic linker's carboxylate (COO^-) groups, while the absorption band around 3400 cm^{-1} was associated with O-H stretching vibrations of adsorbed water molecules. The successful hybrid formation was confirmed by the band at $550\text{--}700\text{ cm}^{-1}$, which indicated the presence of metal-oxygen bonding. XRD analysis showed distinctive diffraction peaks corresponding to the iron-based framework, along with additional peaks associated with NiO and Co_3O_4 , confirming the successful inclusion of Ni and Co species into the MOF structure. The diffraction data matched with JCPDS cards for NiO (01-073-1523), CoO (01-080-1534), and Fe-based MIL-88 (00-034-0529) quite well. The pure MIL-88 showed spindle/rod-like morphology in SEM images. In contrast, the Ni/Co-incorporated sample showed a rougher, more aggregated surface morphology because metal oxide nanoparticles were deposited across the MOF surface. The synthesized materials high surface area and porous character, which provide sufficient active sites for ion diffusion and charge storage, were validated by Brunauer Emmett Teller (BET) analysis. The Ni/Co-incorporated MIL-88 electrode exhibited improved pseudo capacitive behavior, good charge-discharge reversibility, and reduced charge-transfer resistance, as evidenced by electrochemical evaluation using CV, GCD, and EIS.

Hetero-Interfaces in Mn-Co@MIL-100 for High-Performance Supercapacitor Applications

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Metal-organic frameworks (MOFs) such as MIL-100 have attracted significant attention for energy storage applications; however, their limited electrical conductivity restricts their practical performance. In this work, Mn-Co hetero-interfaces were introduced into MIL-100 to enhance its structural and electronic properties. MIL-100 was synthesized via a solvothermal route using ferric nitrate and trimesic acid, while Mn-Co bimetallic nanoparticles were prepared by a co-precipitation method and subsequently incorporated to form Mn-Co@MIL-100 composites. The structural, morphological, and optical properties of the synthesized materials were examined using XRD, SEM, FTIR, BET, and UV-visible spectroscopy. XRD confirmed the successful formation and structural integrity of MIL-100 after modification. SEM revealed morphological changes indicating effective dispersion of Mn-Co nanoparticles within the framework. BET analysis suggested improved surface characteristics and porosity. FTIR confirmed characteristic metal-oxygen and coordinated carboxylate vibrations along with preservation of the framework. UV-Vis spectroscopy indicated electronic interactions between Mn-Co species and MIL-100, confirming hetero-interface formation. Overall, Mn-Co incorporation effectively tailored the physicochemical properties of MIL-100 without destroying its framework, making it a promising candidate for advanced energy storage applications.

Synthesis of a Hierarchical MIL-101/Conducting Polymer Composite for Super Capacitor Application

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Metal Organic Frameworks played a key role in energy applications because of their large pore size, durability, and charge-storing potential. A flexible, high-performance electrode was formed by combining the MIL-101 with conducting polymers. MIL-101 was prepared by a solvothermal method to obtain a highly porous and crystalline framework with a large surface area and tunable pore structure. To enhance electrical conductivity and electrochemical activity, a conducting polymer was uniformly integrated within the MIL-101 framework, forming a hierarchical composite structure with improved charge transport pathways and abundant active sites. The synergistic interaction between the porous MIL-101 matrix and the conducting polymer facilitated efficient ion diffusion and electron transfer, leading to enhanced capacitive performance. The synthesized MIL-101 was successfully confirmed through various characterization techniques. FTIR analysis showed characteristic absorption bands around 3430 cm^{-1} (O–H stretching), 1620 cm^{-1} (C=O stretching), and $560\text{--}750\text{ cm}^{-1}$ corresponding to metal–oxygen vibrations, confirming the successful coordination between metal ions and organic linkers. XRD analysis exhibited sharp diffraction peaks at 2θ values of approximately 5.2° , 8.9° , 9.3° , 16.5° , and 18.7° , indicating the highly crystalline and phase-pure structure of MIL-101. SEM images revealed a well-defined porous morphology with uniformly distributed octahedral particles, while EDX analysis confirmed the presence of major elements such as C, O, and metal species with no significant impurities detected. BET analysis demonstrated a high specific surface area of about $2500\text{--}3200\text{ m}^2\text{ g}^{-1}$ along with a porous framework and large pore volume, which are highly beneficial for efficient electrolyte ion transport and enhanced electrochemical performance in super capacitor applications. Electrochemical measurements, including cyclic voltammetry, galvanostatic charge discharge, and electrochemical impedance spectroscopy, demonstrated improved specific capacitance, rate capability, and cycling stability compared to pristine MIL-101. These results highlight the potential of hierarchical MIL-101/conducting polymer composites as promising electrode materials for next-generation flexible super capacitor applications.

Hetrostructure Ti-doped SnO₂/gC₃N₄ Nanocomposite for Enhance Photocatalytic Degradation of Organic Pollutant and Antibacterial Application

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Water pollution caused by organic dyes, pharmaceuticals, and pathogenic microorganisms poses a significant environmental challenge worldwide. Semiconductor photocatalysis has emerged as a sustainable approach for wastewater treatment due to its ability to utilize solar energy for pollutant degradation. However, pure SnO₂ and g-C₃N₄ suffer from limited visible-light absorption and rapid charge recombination, respectively. The construction of Ti-doped SnO₂/g-C₃N₄ heterostructures offers an effective strategy to enhance photocatalytic and antibacterial performance through improved charge separation and reactive oxygen species generation.

Comparison of Antibacterial Activity of Extract of Leaves of Four *Ziziphus* Species

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Antibacterial destroys bacteria or suppresses their growth or their ability to reproduce. Heat, chemicals such as chlorine, and antibiotic drugs all have antibacterial properties. Different herbs have various useful effect in quire the diseases (antitumor, anti-microbial etc). In this study comparison of such herbs; (*Z.lotus*, *Z.jujube*, *Z.mauritiana*, *Z.spina christi*) that can protect against bacteria. The extract of different herbs were under study (wt range from 10-50g), concentration range was 10-1000 µg/ml. All the herbs shows significant reduction in bacterial efficiency, thereby it is justify that these herbs can work as antibacterial agents. Methanolic extract of *Z. Lotus* possessed maximum significant antibacterial activity with *B. Subtilis*, *Z. jujuba* possessed minimum significant with *P. Aerugenosa* (among these herbs) against, Minimum Inhibitory Concentration Assay when compared to control group. This activity thus lends pharmacological acceptance to the recommended use of *Z. Lotus* as a natural therapy in the treatment of supervision of Antibacterial effects.

Photocatalytic Application of Silver-Coated ZnO Nanoflowers

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This study aims to develop a cost-effective and highly efficient photocatalytic nanomaterial through surface modification and template-assisted synthesis to overcome limitations of conventional photocatalytic systems. ZnO nanoflowers were selected due to their high surface-to-volume ratio and enhanced light scattering properties, which can significantly improve photocatalytic performance. Research Question. Can silver-coated ZnO nanoflowers synthesized on low-cost aluminum substrates enhance photocatalytic efficiency while reducing overall material cost. Silver-coated ZnO nanoflowers were successfully synthesized using a simple hydrothermal approach. Surface modification with Ag nanoparticles significantly enhanced photocatalytic performance by improving charge separation and reducing recombination. Use of low-cost aluminum substrates (98% purity) and carbon electrodes makes the process economical and scalable. Overall, the developed material shows strong potential as an efficient and cost-effective photo catalyst.

Next-Generation Ru/Co Codoped CeNi Bimetallic Nanoparticles with Synergistic Catalytic and Antimicrobial Properties

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The increasing requests for multifunctional nanomaterials capable of treating environmental pollution and antimicrobial resistance have prompted the progress of novel bimetallic nano-hybrids. Herein, we designed a series of next-generation Ru/Co codoped CeNi bimetallic nanoparticles for synergistically enhancing photocatalytic and antibacterial performance through simultaneous modulation of electronic structure and surface characteristics. The development strategy was inspired by recent advances in nanostructured materials that have shown improved electronic transport, tunable surface behavior, and enhanced catalytic performance via nanoscale engineering and compositional modification at the molecular level. The presence of Ru and Co in the CeNi scaffold enhanced charge separation, increased active catalytic sites, diminished electron-hole recombination while accelerating surface reaction dynamics. The successful codoping and enhanced optical properties were confirmed by their structural and physicochemical characterizations, such as XRD, SEM/TEM, EDX mapping, UV-Vis DRS analysis. The characteristic of the photocatalytic activity was performed by methylene blue and rhodamine B removal under visible-light irradiation every 30 minutes, whereas antibacterial property was investigated using *Escherichia coli* and *Staphylococcus aureus*. Kinetic study showed that pseudo-first-order degradation behavior, higher apparent rate constants, lower activation energy values indicated accelerated reaction pathways and facilitated catalytic process. The increased antibacterial activity was due to reactive oxygen species generation, membrane damage and improved interaction between nanoparticles and cells. Ru, Co, Ce and Ni hybridization synergistically resulted in enhanced catalytic efficiency, excellent reaction kinetics and retained reusability. Hence, these findings reveal that Ru/Co codoped CeNi nanoparticles are novel precursors towards eco-friendly environmental remediation technologies, potential biocidal applications and sustainable nanomaterial testing, pioneering multi-functional platforms.

Fabrication of Ru/Co Codoped MoS₂ Nanoparticles for Environmental and Biomedical Applications

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Discharge of organic dyes, industrial pollutants, as well as pathogenic and opportunistic parasites into different water systems are the major issues in many countries leading to environmental and health hazards. However, conventional photocatalysts demonstrate poor visible-light absorption, fast electron-hole recombination and also unsuitable explicit multifunctional performance. In order to overcome these challenges we fabricated Ru/Co codoped MoS₂ nanoparticles with high specific surface area as multivalent nanomaterials for environmental and biomedical applications. This development is based on the potential of dual-metal codoping to synergistically exploit the catalytic and redox efficacy of Ru and Co as compared with single-metal doping. The synthesized nanoparticles have been thoroughly characterized by using a variety of different techniques including XRD, SEM or FESEM, EDX, UV-Vis, and PL. XRD studies confirmed crystal structure and phase purity, SEM showed nanoparticle morphology and surface texture, while EDX provided verification of elemental composition, UV-Vis and PL analyses indicated improved light absorption and reduced charge recombination. Results of photocatalytic degradation indicated rapid degradation of organic dyes, including methylene blue and rhodamine B under light irradiation to show the increased catalytic performance of Ru/Co codoped MoS₂ nanoparticles. Similarly, these nanomaterials are promising also for biomedical applications because of the potential antibacterial property, bioactivity and biocompatibility. For practical applications, future work should optimize the doping ratios, explore real wastewaters for elimination efficiency tests, investigate reusability and stability, cytotoxicity, and antibacterial performance.

Catalytical Applications of Bismuth Based Magnetic Composites

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Bismuth-based magnetic composites are compelling multifunctional catalytic materials owing to their distinctive photocatalytic, magnetic, electrical, and structural properties. Bismuth-containing semiconductors combined with ferrites (e.g., Fe_3O_4 , CoFe_2O_4 , NiFe_2O_4 , and MnFe_2O_4) are favored for addressing environmental and energy challenges. These hybrid materials serve as compelling options for catalysts due to their superior catalytic efficiency, charge carrier separation, magnetic recovery, and chemical stability. Hydrothermal, solvothermal, co-precipitation, sol-gel, combustion, microwave-assisted, and sonochemical methods have been employed to produce nanocomposites with regulated morphology, particle dimensions, and surface characteristics. The catalytic performance of these materials is significantly influenced by their crystal structure, surface area, heterojunction formation, magnetic properties, and the interaction between bismuth semiconductors and magnetic components. Bismuth-based magnetic composites integrate visible-light activity, magnetic separability, chemical stability, and high catalytic efficiency into a singular multifunctional material for sustainable catalysis. Investigations into nanostructure engineering, heterojunction design, defect management, and environmentally friendly synthesis will improve their application in environmental cleanup, renewable energy conversion, and industrial catalysis. These advancements render bismuth-based magnetic composites viable options for efficient, reusable, and eco-friendly catalytic systems that enhance technology and industrial processes.

In Silico Discovery of Novel Zika Virus Inhibitors from Natural Products: An Integrated Study Using DFT, Molecular Docking, and MD Simulations

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The Zika virus (ZIKV) is a mosquito-borne flavivirus has emerged as a major global health problem due to its connection to severe neurological disorders and congenital abnormalities. Although extensive efforts have been made to find an antiviral therapy, there is still no specific antiviral therapy for this virus, which underlines the importance of discovering new antiviral drugs that are effective against relevant viral proteins. For the present study, an integrated in silico study using molecular docking and molecular dynamics (MD) simulations was used to study the potential inhibitory activity of With anolide E against an important ZIKV target protein. The best-ranked docked complex was then subjected to 100ns molecular dynamics (MD) simulations to check the structural stability, conformational flexibility, compactness, solvent accessibility, intermolecular interactions, and binding persistence of the complex. The simulation results showed a dynamic behavior with a lot of conformational adaptation. The backbone and ligand RMSD values were found to be higher for the with anolide E complex for the whole trajectory. None the less, minimum distance values remained and the hydrophobic and hydrogen-bond interactions remained, suggesting continued and effective binding to the active site. RMSF analysis suggested that fluctuations were mostly limited to loop and terminal regions whereas the core residues of the target protein maintained structural rigidity. In summary, the results indicate an appreciable protein–ligand contact network, which was also stable and persistent throughout the simulation, for interaction between with anolide E and the ZIKV target protein. The results serve as an excellent computational foundation for the continued experimental evaluation of with anolide E as anti-ZIKV agent.

Novel Inhibitors of Nipah Virus Discovery by in Silico Approach: DFT, Molecular Docking, and MD Simulation Approaches.

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The Nipah virus (NiV) is part of the family Mononegavirales, is highly virulent, high mortality and currently there is no approved vaccine or specific antiviral drugs. The receptor that the attachment glycoprotein (G) binds to is the human ephrinB2 receptor and thus is a key player for viral entry. To address this therapeutic void, a systematic in silico study was carried out to identify novel NiV inhibitors by natural compound databases, where compounds with novel structures and the best PK profile were selected. The method has been a hierarchy computation process. The pharmacological profiling was carried out at the SwissADME laboratory, which led to a preliminary screening of selected phytochemicals, where the drug-like properties were favourable and strict adherence to Lipinski's Rule of Five. The large-scale molecular docking done with Auto Dock Vina revealed that with anolide E is the best fit with a binding affinity of -9.16 kcal/mol towards NiV G–ephrinB2 complex (PDB ID: 2VSM). The reactivity of the chemicals and Electronic stability were calculated by Density Functional Theory (DFT) method at B3LYP/6-31G (d,p) level. The energy of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), of withanolide E was determined to be -6.55 eV and -1.42 eV, respectively. This gives rise to a large energy gap between the HOMO and LUMO (5.13 eV), that is well consistent with the electronic stability, optimal chemical hardness and resistance to off-target biochemical degradation. This dynamic ability of the top compound was further tested and validated by running a 100ns Molecular Dynamics (MD) simulation. Trajectory analysis was used to check the decent structural stability and Root Mean Square Deviation (RMSD) of protein backbone was found to be increasing towards a compact structure. It was confirmed by the intermolecular hydrogen-bonding interactions and a stable solvent accessible surface area (SASA) was calculated over 100 ns time scale. Ultimately, this study recognises with anolide E as a highly encouraging support for developing novel antiviral agents to block Nipah virus entry.

Sustainable Aviation Fuel Production by Catalytic Hydrocracking of Tobacco Seeds Oil over Modified Clay

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The global aviation industry is responsible for environmental emissions such as greenhouse gas GHG. Nowadays, this sector is responsible for approximately 2-3% of anthropogenic CO₂ emissions, with expectations that indicate a 300-700% rise in demand by 2050 in comparison to 2005. Additionally, aviation also has a 13.9% share of the transport sector and has now become the second-highest source of GHG emissions, after road transport. To solve this problem, sustainable aviation fuels (SAFs) are used instead of fossil fuels. Because SAFs are known to be renewable substitutes for conventional jet fuel. They are made from non-petroleum-based feedstocks such as non-edible oils, vegetable oils, agricultural and forestry waste. In this research, tobacco seed oil (TSO) is used as a feedstock to produce SAF by hydrocracking over HCl-modified bentonite clay. For modification, bentonite clay is treated with 0.1M HCl to 4h in a Soxhlet apparatus, then washed, filtered, dried, and powdered. Then used as a catalyst for TSO hydrocracking in a closed system at high temperature and pressure. the modified catalyst is characterized by SEM-EDX, and XRD. While the resultant product of hydrocracking is characterized by GC-MS to confirm the production of jet biofuel from TSO.

