

APRIL 14th-15th, 2025

# **Abstract Book**







## Welcome to ICONN-2025

On behalf of the organizing committee, I am delighted and honored to welcome all the guests, speakers and the participants of the 3rd International Conference on Nanoscience & Nanotechnology (ICONN-2025). ICONN is a joint venture of the School of Chemical and Materials Engineering (SCME), National University of Sciences & Technology (NUST), Islamabad and Department of Chemistry & Chemical



Engineering, SBA School of Science & Engineering, Lahore University of Management Sciences (LUMS). The first conference (ICONN-2018) of this series was successfully held at SCME, NUST on Nov. 1-2, 2018, while the second conference of this series was held at the LUMS on Nov. 1-2, 2019. This year, we are also collaborating with Dr. NM Butt (Felow Pakistan Academy of Sciences & former Chairman Pakistan Science Foundation, presently at the Preston Institute of Nano Science & Technology (PINSAT), Islamabad) and Prof. Dr. M. Mujahid (Pak-Austria Fachhochschule, Institute of Applied Sciences & Technology, Mang, Haripur, KPK). The major focus of ICONN-2025 is to highlight the important developments made in nanomaterials research, especially in the synthesis, fabrication and applications of nanomaterials in biomedical sciences (biosensors, LoC devices), renewable energy technologies (energy storage and conversions) and the environment (catalysis, separation devices). In addition to the keynote/invited speakers from Pakistan (10) and abroad (12) and SCME students, over 120 participants have been registered for this conference from academia and industry. Furthermore, a poster session is being organized to offer a platform to the students/young researchers to showcase their research in the field of Nanoscience & Nanotechnology. ICONN-2025 will provide an exciting opportunity for the young researchers for networking and for future collaboration with the national/international leading research groups to collectively explore new and exciting avenues in the emerging and multidisciplinary field of Nanoscience & Nanotechnology. Organizing such an event in the resources limited environment was a huge undertaking and hence I thank SCME organizing committee/staff/students and our partners from LUMS, Preston, PAF-IAST for their unwavering support. On behalf of the organizing committee, I also acknowledge the support from various sponsors especially NUST, HEC, COMSTECH, Pakistan Academy of Sciences, Pakistan Science Foundation, education professional consultants, PPG, E-Triangle Automation, Science Centre, Pak Glorious, A&S enterprises and Aamir & Sons. We wish all the participants of ICONN-2025 an amazing and productive stay at NUST.

## Prof. Dr. Zakir Hussain

Co-Organizer ICONN-2025 (SCME-NUST)

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#### Nano-electrodeposition

Dr. Walther Schwarzacher

Dean, Syed Babar Ali School of Science and Engineering, LUMS, Lahore

**Abstract:** Metal electrodeposition will contribute to a zero-carbon future through its roles in rechargeable batteries, electrocatalyst production, and resource conservation through corrosion protection. This presentation focuses on Ni electrodeposition, firstly to understand how the morphology of a polycrystalline Ni film evolves during growth, and secondly to investigate the growth of short-period Ni/Cu multilayers on various substrates. For the former, we apply a combination of atomic force microscopy and scanning electron microscopy with slope and textural analysis. For Ni/Cu multilayers, a system that has been widely studied using aqueous electrolytes, we show that non-aqueous ethaline (1:2 choline chloride : ethylene glycol) is a promising alternative.

## Nanostructures as Novel Drug Delivery Systems: Fundamental Issues and Market Perspectives

#### Dr. Rassoul Dinarvand

Professor of Pharmaceutics and Director, Nanotechnology Research Centre, Tehran University of Medical Sciences, Iran.

Abstract: Nanostructures have been the forefront of transformation of drug delivery systems, offering unprecedented precision and efficacy. This presentation delves into the importance of nanomedicine and its pivotal role in addressing critical health challenges, focusing mainly on cancer therapy. Nanomedicine improves the targeting of therapies, minimizes adverse side effects, and has opened avenues to treat complex diseases like cancer and neurodegenerative disorders. The talk explores the diverse types of nanomedicines currently in development and use, such as polymeric nanoparticles, lipid-based nanoparticles, and antibody-drug conjugates. Each type is examined in terms of structure, functionality, and its application in various therapeutic areas. Polymeric nanoparticles stand out for their versatility in encapsulating drugs and enabling controlled/targeted release, while lipid-based nanoparticles have gained significant traction, particularly in the delivery of genetic material, such as nucleotides. Antibody-drug conjugates represent the cutting-edge innovation, combining the specificity of monoclonal antibodies with potent therapeutic agents, ensuring precise targeting of pathological cells. Moreover, the mechanisms by which nanomedicine enhances anticancer efficacy and reduces side effects are thoroughly discussed. These mechanisms include improved bioavailability, enhanced cellular uptake, and targeted delivery systems that focus on tumor microenvironments. These advances not only maximize therapeutic benefits but also reduce systemic toxicity, a major drawback of conventional cancer treatments. The presentation also ventures into market perspectives, shedding light on the challenges and opportunities in commercializing nanomedicine. While the promise of nanostructures in drug delivery is undeniable, issues such as regulatory approval, production scalability, and cost-effectiveness need to be addressed to ensure broader market adoption. Nevertheless, the rapid advancements in nanotechnology, coupled with growing investments in research and development, indicate a bright future for nanomedicine as a transformative force in healthcare. This comprehensive overview aims to bridge the fundamental scientific principles of nanomedicine with its practical and market implications. This presentation seeks to inspire continued innovation and collaboration in this exciting and impactful field.

#### PS-2

## Microorganisms in the LED spotlight: Light-Assisted Biosynthesis of Valuable Substances

## Dr. Harald Schoebel

Department Biotechnology, MCI| The Entrepreneurial School® Innsbruck, Austria

**Abstract:** Physical-chemical parameters play a crucial role in the modification and optimization of biotechnological processes. For phototrophic microorganisms such as microalgae, light can be one such critical parameter. It serves as an energy source for photosynthesis and influences secondary metabolism. However, the effect of light on metabolism is not limited to phototrophic organisms. The induction or enhancement of secondary metabolite production can also be observed in fungi and bacteria. Varying light conditions in terms of wavelength and irradiance is therefore a promising approach to optimizing biotechnological processes.

The rapid development of LED technology enables the development of flexible and customized irradiation systems. As a result, LEDs are playing an increasingly important role in the cultivation processes and thus in the biotechnological production of valuable substances. This presentation will explore how LED-based irradiation systems influence biotechnological processes, focusing on how lighting scenarios can be specifically adapted and optimized for light-related experiments and characterized in a standardized manner. In addition, the induction and modification of metal nanoparticle biosynthesis by targeted light irradiation will be analyzed.

Illumination systems for light-based biotechnology experiments require accurate and reproducible characterization of light parameters such as irradiance and photon flux density. This can be challenging due to complex experimental setups. Optical simulations using ray-tracing software offer a solution by complementing direct measurements and providing additional insight into the light distribution. This presentation will provide a brief introduction to modeling life science experiments using ray-tracing software, and will be illustrated with selected case studies. Simulated irradiance distributions in UV inactivation studies and light stress experiments with microalgae will be compared to optical measurements. In addition, optical methods for optimizing irradiation conditions in applications such as photobioreactors and screening systems are discussed, highlighting their potential for achieving uniform light distributions.

The biobased production of metal nanoparticles offers a sustainable alternative to commercially used physico-chemical production processes, yielding high-quality nanomaterials with narrow size distributions, high stability, and biocompatibility, all with broad application potential. The intrinsic properties of nanoparticles depend on their size and shape, which can be controlled through manufacturing parameters. This presentation will explore the potential of microalgae for the biosynthesis of gold and silver nanoparticles. Extracts from different microalgal strains were used to study metal nanoparticle synthesis under variable light conditions. It was found that light can enhance synthesis rates, and for some algal strains, nanoparticle synthesis would not be possible without light.

Additionally, this presentation will discuss the modification of silver nanoparticle biosynthesis using the yeast strain Saccharomyces cerevisiae. Single-parameter optimization strategies were applied during cultivation, extraction, and synthesis to control nanoparticle size and yield. Visible light was a key factor in nanoparticle production. The effect of white light on silver nanoparticle biosynthesis was investigated using advanced LED systems with different irradiation intensities, alongside dark control experiments. Spectrophotometric analysis, dynamic light scattering, scanning electron microscopy, and energy-dispersive X-ray spectroscopy confirmed the formation of spherical silver nanoparticles with light-mediated size modulation and significantly increased yields. Comparison of irradiated and non-irradiated samples highlighted the critical role of photon input and the high sensitivity of the biosynthetic process. Irradiation led to a more than 90% increase in nanoparticle yield and a significant reduction in particle sizes of 130 nm and 100 nm, respectively. These results establish white light as a powerful tool for nanomanufacturing, enabling precise control over nanoparticle properties.

# Functionalising Thiosemicarbazones for Covalent Immobilisation on Nanoparticles and More

Johannes Hohnsen, Axel Klein

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#### **Background and aims**

Thiosemicarbazones (TSC) (Scheme 1) are a versatile class of molecules with established antibiological properties. Their medical application is frequently hampered through their pronounced lipophilic character. Approaches towards their applicability are their controlled release from metal complexes, from mesoporous materials, and from polymers, the build-up of TSC-peptide conjugates for their cell-incorporation, and their binding to nanoparticle (NP) surfaces. The aim of this research project is the vast use of TSC as multifunctional units in NP conjugates. The advantage of TSC is the vast chemical variability through the four substituents R to R<sup>\*\*</sup>.



**Scheme 1.** A: Thiosemicarbazones (TSC) in their thione or thiol form (with numbering); B: Metisazone, an approved drug against small pox; C: Dp44mT a topoisomerase inhibitor; **D**: TSC as functional groups in NP-conjugates.

#### Methods

The approach to use TSC as functional units in conjugates with applications in biomedicine and other fields require the mastering of the chemistry of the anchoring, functional, and conjugating groups (Scheme 1D). TSC provide the benefit that the formation reaction from carbonyl-containing molecules (bearing R and R') and thiosemicarbazides (bearing R" and R"") is simple and allows modular synthesis of various derivatives.



Scheme 2. A: Modular synthesis of TSCs.; B: Composition of thiosemicarbazides.

#### **Results**

The R and R' substitution of TSC (Scheme 1A) was used to introduce further coordinating functions, fluorophores such as anthracenyl and to enhance the toxicity of TSC by introducing the dipyridyl function (Scheme 1C). In the *N*4 position we were able to introduce various conjugating groups such as CN, alkynes, esters, amines, but also anchoring functions such as carboxylates, phosphonates, and thiolates tailored for various nanoparticle surfaces such as SiO<sub>2</sub>, Fe<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, Au, and more.

#### IIT-2

#### Conclusion

We have worked out strategies to vary all four substituents on TSC with the aim of providing the necessary chemistry for an extensive use of TSC units in NP conjugates connecting NP to various chemical (e.g. coordinating), physicochemical (e.g. luminescent), and biochemical functions (e.g. cell penetrating peptides). Furthermore, TSCs themselves can be useful as both metal-coordinating and cytotoxic entities in such conjugates.

#### From Waste to Valuable: Nanomaterials for Sustainable Environment

### Dr. M. Nawaz Tahir

## Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia

Abstract: The increasing accumulation of waste polymers (plastic and biomass) in our ecosystem, largely driven by the industrial revolution, has sparked significant concerns about environmental sustainability. Additionally, energy systems reliant on fossil fuels pose a major threat to the planet, primarily due to the excessive emission of greenhouse gases into the atmosphere. To tackle these issues, there is an urgent need to develop technologies that facilitate a smooth transition away from fossil-based fuels and enable effective management of polymer waste. In this context, among the various renewable energy options, solar energy conversion is leading the way. The direct beam solar radiation surpasses the global human energy consumption (25,300 terawatt-hours in 2021). Additionally, the chemical energy stored in waste polymers can be utilized to not only boost renewable energy production but also generate valuable byproducts, contributing to a circular economy. A promising strategy involves the photo/electro reforming of waste polymers to produce useful products, alongside the splitting of water to produce green hydrogen fuel (H<sub>2</sub>), addressing two critical issues at once. As waste polymers, water, and solar energy are abundant resources, the key to unlocking their full potential lies in the development of efficient photo/electrocatalysts. The nanomaterials with exceptional physicochemical properties could be the potential for next generation photo/electrocatalysts. In this contribution, we focused on the synthesis and characterization of photo/electrocatalysts in the nanometer size regime, using waste polymers either as precursor materials or sacrificial agents to boost green hydrogen fuel production and fien chemicals, thus contributing to environmental sustainability. We have developed low-cost, transition metaldoped metal oxides (e.g., Ta, W, Mo) or 2D polymeric carbon nitrides (with molecular formulas C<sub>3</sub>N<sub>4</sub> and C<sub>3</sub>N<sub>3</sub>), which possess tailored optical, electronic, and chemical properties. To enhance the performance of these low-cost and environmentally friendly photo/electrocatalysts, we have combined them with highly reduced graphene oxide or metal phosphides. These photo/-electrocatalysts have been successfully employed to generate green hydrogen fuel and organic fine chemicals

## Engineering Particles via Flash Nanoprecipitation for Applications in Biomedicine

Dr. Sulalit Bandyopadhyay

Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

**Abstract:** Magnetic monodomain iron oxide nanoparticles (IONPs) find wide biomedical applications ranging from diagnostics to therapeutics such as in magnetic hyperthermia, targeted drug delivery, etc. Their performance in such applications is governed by their magnetic properties which in turn are influenced by particle size, shape, inter particle interactions among others. IONPs synthesized via thermal decomposition of iron – oleate, pentacarbonyl, etc in organic solvents leads to precise control of size, size distribution, magnetic properties when compared to IONPs synthesized via co-precipitation. However, for biomedical applications, these IONPs should be water dispersible - phase transfer also introduces other caveats such as aggregation, reduction in magnetic properties and so on. While water dispersibility is not a challenge for the co-precipitation IONPs, to tailor the particles towards specific applications, post functionalization is an important subsequent step.

This talk will focus on a novel flash nanoprecipitation (FNP) technique that has been tuned to both (i) functionalize IONPs synthesized via thermal decomposition whereby facilitating phase transfer and polymer encapsulation simultaneously and (ii) coat hydrophilic IONPs synthesized via co-precipitation via hydrophobic ion-pairing. A close mapping of operational parameters and system constituents of the FNP process on the resultant physico-chemical properties of the polymer encapsulated IONPs will be presented, followed by their applications in the field of drug delivery among others.

## Water-Surface Interactions in Nanoporous Materials

Dr. Christian Weinberger

Akademischer Oberrat Inorganic Functional Materials, Paderborn University, Germany

**Abstract:** Water–surface interactions play a crucial role in energy-related applications, such as adsorption-based heat pumps. Achieving the appropriate interaction strength is essential for reversible adsorption-desorption dynamics, which in turn enables efficient system performance. Therefore, the ability to fine-tune interactions between adsorbate and adsorbent emerges as a key requirement. Porous materials offer unique advantages in this regard, including high specific surface area, adjustable pore sizes, and tunable surface chemistry, making them ideal model systems for studying water–surface interactions.

In this study, we investigate the Metal-Organic Framework (MOF) type CPO-27 (also known as MOF-74), which features divalent metal centres and 2,5-dihydroxyterephthalate as the linker molecule. This framework crystallizes in a honeycomb-like structure, resulting in well-defined cylindrical pores. By systematically varying the metal centre and linker type, we demonstrate the impact of framework chemistry on water sorption behaviour and interaction strength.

Furthermore, porous silica materials with different surface functionalities are examined to illustrate how chemical surface modifications influence surface polarity. This comparative approach allows us to derive general principles for tailoring water–surface interactions across different classes of porous materials.

We present a comprehensive overview of the critical parameters that can be tuned for modulating surface polarity and controlling adsorption behaviour. To elucidate the underlying interaction mechanisms, we combine water sorption measurements, infrared spectroscopy, and molecular dynamics simulations. These complementary methods provide both macroscopic and molecular-scale insights, enabling a deeper understanding of how surface chemistry governs water sorption in porous frameworks.

# Fabrication of Dye-Sensitized Solar Cells Using Natural Materials For Powering IOT Devices

#### Dr. Muhammad Awais

Department of Industrial Engineering, Taibah University, Medina, Saudi Arabia

Abstract: Dye-sensitized solar cells (DSSCs) are a third-generation technology for converting solar radiation into electrical energy. These cells are economically viable owing to the utilization of cost-effective materials and simplified manufacturing processes. They present a promising solution for sustainable energy production, particularly in indoor environments under ambient illumination. DSSCs comprise four essential components: a TiO<sub>2</sub> working electrode, graphite counter electrode, triiodide/iodide electrolyte, and light-absorbing dye. This investigation focuses on the synthesis of light-absorbing dyes from readily accessible natural sources, including plant and fruit extracts. Various botanical specimens such as Cardamom, Henna, Turmeric, Cumin, Saffron, and Black tea, along with fruit extracts including Ajwa, Beet, Pomegranate, Tamarind, and Cacao, have been employed as dyes in DSSC fabrication. These extracts underwent water solubilization, and the working electrodes were prepared by immersing TiO<sub>2</sub> glass electrodes in these solutions for a predetermined duration. A design of experiment investigation was conducted to explore the relationship between factors influencing the selection of optimal natural materials or combinations for DSSC dye production. The assembled DSSCs were evaluated under solar irradiation by measuring their voltage outputs, and the highest-performing dyes were identified. This research highlights the potential of natural materials for indoor energy harvesting applications, particularly in powering Internet of Things (IoT) devices, thus advancing renewable energy and sustainable technology integration.

## Developing Eco-Friendly and Efficient Mesoporous Hybrid Materials For Environmental Applications

#### Dr. Mohamed A. Shenashen

Professor of Materials Science, Department of Petrochemical, Egyptian Petroleum Research Institute (EPRI), Nasr City, Cairo, Egypt

Abstract: A major concern in modern society is the availability of robust technology to fulfill daily demands and maintain a tranquil existence. The remarkable functional features of nanostructured materials have revolutionized a wide range of scientific domains, including electronics, biology, optics, and catalysis. Particularly notable are mesoporous materials, whose unique structural properties allow for innovative uses in a variety of applications. The development of effective and eco-friendly hybrid mesoporous nanomaterials is a groundbreaking strategy for addressing pressing environmental issues. Utilizing the distinctive properties of hybrid mesoporous materials, these materials are made to carry out specific environmental tasks such as resource recovery, adsorption, and sensing. Their outstanding structural features, including expansive surface areas, adjustable pore structures, and multifunctional capabilities, make them exceptionally effective for environmental pollution mitigation, rare and precious metal recovery, and hazardous material detection and removal. Our research responds to the growing demand for sustainable technologies by developing costeffective, eco-friendly, mesoporous nanomaterials with potential applications in the energy, healthcare, and environmental sectors. Through the integration of creative design methodologies and green chemistry concepts, the designed mesoporous materials offer viable solutions to urgent environmental and economic issues. Furthermore, these hybrid mesoporous materials demonstrate outstanding potential as biosensors for healthcare monitoring and as electrodes in energy devices, highlighting their versatility in multiple fields. The development of mesoporous hybrid nanomaterials promotes sustainable solutions that align with global environmental objectives, foster a cleaner and more efficient use of resources, and connect material innovation with real-world applications.

## Controllable Preparation and Oxygen Reduction Application of Non-Noble Metal Nanocomposites

Dr. Xiaoxiao Huang

Department of Physics, Beijing Normal University, China

**Abstract:** Recently, carbonized metal-organic frameworks (MOFs) with abundant transition active sites have been explored with impressive oxygen electro-catalytic performance. However, an activity gap still exists between the traditional MOFs-derived catalysts and noble-metal catalysts and the precise active sites modulation also need to be developed. Herein, we further advance currently prevalent M/N-C based nanomaterials via simultaneous controls in morphology and architecture as highly efficient oxygen electro-catalysts, which present highly active oxygen catalytic performance. The mechanism of active sites working and decaying is also be explored.

## Design of Profiles in Batch Processes and CFD Simulations With Direct Inverse Analysis of Machine Learning Models

#### Dr. Hiromasa Kaneko

## Department of Applied Chemistry, School of Science and Technology, Meiji University, Kanagawa, Japan

Abstract: In molecular, material, and process designs, it is important to perform inverse analysis of mathematical models constructed with machine learning using target values of the properties and activities. While many approaches employ a pseudo-inverse analysis, Gaussian mixture regression (GMR) can achieve direct inverse analysis. Although Bayesian optimization (BO) is an effective tool, BO merely selects a candidate from a limited number of samples, and the samples do not necessarily contain the optimal solution. Furthermore, because upper and lower limits are set for explanatory variables x, it is not possible to obtain solutions that go beyond these limits. To solve these issues, direct inverse analysis of the GMR model was proposed because GMR models can estimate x values directly based on the target values of objective variables y. The proposed method could allow the target y value to be achieved with a dramatically smaller number of experiments than by BO, especially when the number of xvariables was large. Furthermore, the proposed direct inverse analysis was applied to timeseries data analysis and process design, and could design both the batch time and the process variable profiles to ensure that the endpoints, such as the product quality and the material properties, possess the target values following a batch process. Then, the proposed method was applied to predict CFD simulation results and design process conditions for the optimization of CFD simulation results (Ind. Eng. Chem. Res. (2025) 3937).

## Novel Nanostructured Metal Oxide Materials For Applications in Solar Cells and Molecular Separation

## Dr. Jan-Henrik Smått

Laboratory of Molecular Science and Engineering, Åbo Akademi University, Henriksgatan 2, 20500 Turku, Finland.

**Abstract:** Cost-efficient solution processing can be used to prepare a range of nanostructured metal oxide materials. For instance, sol-gel processing combined with supramolecular templating can be used to produce nanoporous  $SiO_2$  and  $TiO_2$  materials of different morphology (e.g., nanoparticles, thin films, and bulk materials). Furthermore, the nanocasting approach can then be used to further replicate these structures into carbon and other metal oxides (SnO2, In<sub>2</sub>O<sub>3</sub>, Co<sub>3</sub>O<sub>4</sub>, ZnO, etc.) with similar porosity and morphology.

The hierarchically structured metal oxides can be utilized in molecular separation applications (including liquid chromatography, phosphopeptide enrichment, and in-tube extraction) as well as in gas sensing. The selectivity towards certain chemical compounds arises from the unique acid-base properties of the metal oxides. We are currently investigating such molecular interactions using nanoplasmonic sensing, which is a powerful tool for studying adsorption kinetics, binding strength, and diffusion of molecules.

Furthermore, sol-gel-derived metal oxides can also be utilized in many types of thin film solar cells (e.g., dye-sensitized, organic, and perovskite solar cells). For instance, the dip coating method can be used to prepare uniform TiO2 thin films with controllable thickness and porosity for applications as charge selective layers in organic and perovskite solar cells. The general focus of our research is to clarify how different deposition methods, type of metal oxide, structural properties, and illumination affect the charge selectivity mechanism in these metal oxides.

## Lightweight Multifunctional Structural Composites

Dr. Pagona Papakonstantinou

School of Engineering, Ulster University, United Kingdom

**Abstract:** In recent years we have seen a gradual migration in airplanes, trains and cars from metallic to composite structures, (mainly Carbon Fibre Reinforced Polymers, CFRP), driven by new requirements for cost efficiency and ecological policies for more environmentally friendly infrastructure by year 2050. A plausible solution to meet these ever increasing requirements is to render the composites multifunctional.

For example, in today's state of the art vehicles, functions such as energy storage, are provided by embedded components (e.g. batteries, supercapacitors), which add significant weight and volume to the vehicle. A nature inspired approach to tackle this challenge is one in which the desired functions are built into constituent structural materials (fibres and polymers) without parasitic parts, rendering the overall system multifunctional. If the body of a vehicle could be replaced with a multifunctional material that would serve simultaneously as both the vehicle structure (i.e. crash absorber or load carrying part) and an energy storage material, significant performance enhancements could be achieved. This multifunctional approach requires electrodes and/or electrolytes that do not only store electrochemical energy but also impart mechanical integrity.

In the talk, I will discuss our recent results on multifunctional structural supercapacitors (SS), which are based on carbon fiber electrodes with radially aligned graphene nanoflakes directly grown on them. I will also emphasize the importance of interfacial nano-engineering on the design of next generation multifunctional fiber reinforced composites.

## Nano-Biosensors: Transforming Diagnosis and Management Tool in Healthcare

## Dr. Mahmood Hassan Akhtar

Hangzhou Zheda Dixun Biological Gene Engineering Co., Ltd. Hangzhou (Zhejiang), China

Abstract: According to the World Health Organization (WHO), neurological disorders (NDs), which affect the central and peripheral nervous systems, impact millions of people globally, posing significant challenges to healthcare systems. These conditions, ranging from Alzheimer's disease to epilepsy and Parkinson's disease to psychiatric disorders, are often complex and require early detection and personalized treatment strategies for effective management. In this context, emerging diagnostic approaches, such as multi-omics technologies and wearable biosensors, are revolutionizing the field. Advancements in nanotechnology have enabled the development of state-of-the-art chip-based diagnostic tools, offering unparalleled precision, sensitivity, and real-time monitoring capabilities. Nanobiosensors can detect biomarkers at ultra-low concentrations, facilitating early diagnosis and tailored therapeutic interventions. Their integration into healthcare systems enhances diagnostic accuracy while enabling continuous patient monitoring, providing data-driven insights for better disease management. The application of nano-biosensors in neurological disorders represents a transformative shift in medical diagnosis and care. By enabling early detection and personalized treatment, they empower patients through real-time health monitoring, fostering a proactive approach to disease management. This technological advancement holds immense potential to bridge gaps in neurological care, offering a holistic, patient-centered approach to managing these debilitating conditions. By leveraging nanobiosensors, we can enhance the quality of life for patients worldwide, paving the way for a new era in neurology and healthcare innovation.

## The Design & Development of Multifaceted Scaffolds for Enhanced Guided Hard Tissue Engineering

## Dr. Ather Farooq Khan

Interdisciplinary Research Centre in Biomedical Materials, COMSATS University Islamabad, Lahore campus, Lahore, Pakistan

Abstract: The main aim of tissue engineering is to develop tailored materials that can promote the regeneration of damaged tissue. This process often involves multiple tissue layers with distinct cellular functions and molecular structures. To achieve this goal we have been working on developing scaffolds that can provide cues for region-specific properties that can help in better growth of tissues. Multilayered scaffolds were designed for use in various tissue engineering applications, including dura mater regeneration, periosteum regeneration, alveolar bone regeneration and periodontium regeneration. The scaffolds were thoroughly characterized for their physical and chemical properties, including porosity, degradation rate, mechanical strength and surface morphology. We have also evaluated the scaffolds' biocompatibility through detailed cell culture studies assessing cell attachment, proliferation and migration. The findings of these studies suggested that these multilayered composite scaffolds can be excellent candidates for tissue engineering applications.

## Covalent Conjugates of Polymers For Addressing Energy and Environmental Challenges

Dr. Basit Yameen

Department of Chemistry and Chemical Engineering, Lahore University of Management Sciences (LUMS), Lahore, Pakistan

Abstract: Covalent conjugates of polymers have emerged as a convenient tool for achieving a variety of functional materials. The key advantages of such constructs include their physical robustness and chemical stability. In addition, the provision of a high degree of synthetic flexibility towards the introduction of a variety of functional groups has made such constructs attractive for the fabrication of materials with controlled properties for a diverse range of applications. The scope and relevance of the polymer based covalent constructs for developing materials with controlled and unique properties for applications in the fields ranging from environment to energy will be presented. The discussion will encompass our work related to the development of novel polymer-based constructs for addressing environment and energy related challenges. 1) 2) Sana Iqbal, Ammar Ahmed Khan, Nauman Zaffar Butt, Raja Shahid Ashraf, and Basit Yameen\*, "All organic double cable polymers of polythiophene donor with rhodanine and perylene diimide acceptors and evaluation of photocurrent generation" Journal of Materials Chemistry C, 2023, 11, 16037-16048. Sunniya Iftikhar, Saba Aslam, Hatice Duran, Senem Çitoğlu, Katrin Kirchhoff, Ingo Lieberwirth, Manzar Sohail, Basit Yameen\*, "Poly(3 hexylthiophene) stabilized ultrafine nickel oxide nanoparticles as superior electrocatalyst for oxygen evolution reaction: Catalyst design through synergistic combination of  $\pi$ -conjugated polymers and metal-based nanoparticles" Journal of Applied Polymer Science, 2022, e52636. 3) Sunniya Iftikhar, Nauman Zafar Butt, Raja Shahid Ashraf, Basit Yameen\*, "Prato Reaction Derived Polythiophene/C60 Donor-Acceptor Double Cable Polymer, Fabrication of Photodetectors and Evaluation of Photocurrent Generation" Journal of Materials Chemistry C, 2020, 8, 17365-17373.

## Two-Dimensional Materials: A New Class for Water Purification and Desalination Technologies

## Dr. Khalid Hussain Thebo

Shenyang National Laboratory for Materials Science, Chinese Academy of Sciences, Shenyang, China/ NESCOM, Islamabad, Pakistan

**Abstract:** Membrane-based technology plays a significant role in environmental remediation and clean energy applications. Recently, two-dimensional (2D) materials of atomic thickness have emerged as nano-building blocks to develop high-performance separation membranes that feature unique nanopores and/or nanochannels. These 2D-material membranes exhibit extraordinary permeation properties, opening a new avenue for ultra-fast and highly selective membranes. However, it is still very challenging to further improve the water permeability without sacrificing the separation efficiency, and such membranes are not stable in an aqueous environment. In my talk, I shall discuss various synthesis and modification methods of 2D materials and their utilization in water filtration and desalination applications.

## Quantum Breakthroughs: Applications and Global Market of Energy-Efficient High-Frequency Quantum Semiconductor Devices

## Dr. Muhammad Usman

Faculty of Engineering Sciences, Ghulam Ishaq Khan Institute of Engineering Sciences and Technology, Topi, Swabi, KPK, Pakistan

Abstract: The Quantum Engineering Group at Ghulam Ishaq Khan Institute of Engineering Sciences and Technology, Pakistan, is at the forefront of pioneering research in III-V-based light-emitting diodes (LEDs), laser diodes, and high electron mobility transistors (HEMTs). Our extensive research portfolio encompasses a diverse range of cutting-edge technologies, including wide bandgap materials and devices, quantum wells and quantum devices, solid-state lighting, energy harvesting, storage and conservation, and visible light communication (VLC). These innovations hold transformative potential for multiple global industries. Solid-state lighting and quantum devices contribute significantly to the LED and laser diode markets, projected to reach a global market size of USD 151.02 billion by 2027. These technologies promise energy efficiency, extended lifespans, and enhanced performance in commercial, residential, and industrial lighting. The visible light communication market is anticipated to grow to USD 113.27 billion by 2030, driven by demand for secure, high-bandwidth communication in smart cities, healthcare, and consumer electronics. By addressing these critical areas, our research not only contributes to technological advancements but also drives significant economic growth in global markets. Our innovative solutions have the potential to revolutionize industries, create new market opportunities, and improve the quality of life worldwide.

## Machine Learning Algorithms for Predicting Band Gaps and Photocatalysis Applications of Semiconductor Nanomaterials

## Dr. Muhammad Akhyar Farrukh

Department of Basic and Applied Chemistry, Faculty of Science and Technology, University of Central Punjab, Lahore, Pakistan

**Abstract:** Artificial Intelligence (AI) refers to the simulation of human intelligence in machines while characterization of nanomaterials by molecular spectroscopy helps in the deep leaning. In this way, we can get Big Data by comparing results with multiple techniques. AI and Big Data are highly interconnected and often work together to automate decision-making processes and pattern recognition because Big Data provides the volume and variety of data needed to identify complex patterns.

Big data can be collected for synthesis and analysis of nanomaterials to develop AI-integrated system, which will be able to determine best reaction parameters for the synthesis and characterization with high accuracy of variety of nanomaterials with less time. Molecular spectroscopy was used in characterization of nanomaterials to develop AI-integrated analysis. While Big Data was collected by different characterization techniques like, Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC) Fourier Transform-Infrared Spectroscopy (FTIR), Particle Size Analyzer (PSA), Powder X-ray Diffraction (XRD), Flame Emission Scanning Electron Microscopy (FESEM), Energy Dispersive X-ray (EDX), High Resolution Transmission Electron Microscopy (HRTEM), Photoluminescence (PL) and Ultraviolet-Visible spectrophotometer (UV-VIS).

We have successfully synthesized more than 65 nanocomposites with variety of metals and metal oxides nanoparticles including p, d and f block elements along with derivative of graphene. Different synthetic routes have been used while green synthesis is sustainable, environmentally eco-friendly method which helps to eliminate toxic waste.

Narrow band gap semiconductors have many industrial applications in sensor, solar cells, solid oxide fuel cells, photovoltaic, batteries photocatalytic degradations of pollutants coming out from textile, pharmaceutical, pesticides, and chemical industries. Machine Learning Algorithms were used to train and test the model for prediction of band gap calculations.

## Quantum Modelling of Multi-Directional Fused-Ring Electron Acceptors For Organic Photovoltaics

## Dr. Raja Shahid Ashraf

### Department of Chemistry, GCU, Lahore, Pakistan

Abstract: Multi-directional fused-ring electron acceptors (FREAs) feature a fused-ring backbone that extends in multiple directions through bridging and acceptor units. This unique structural design imparts several advantageous properties, like increased light absorption, precise energy level adjustments, improved electron mobility, reduced energy loss, and enhanced efficiency in organic photovoltaic (OPV) devices. In this study, we designed seven novel multi-directional FREAs and conducted a comprehensive computational analysis using Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT). The designed molecules feature a benzotrithienopyrrole central core connected to a  $\pi$ -bridge acceptor, either benzothiadiazole or benzotriazole, and three varying terminal acceptors, including malononitrile, 2-(5,6-difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile, and 2-(3methyl-4-oxothiazolidin-2-ylidene)malononitrile. Our investigation encompassed the evaluation of geometry, frontier molecular orbitals (FMOs), optical properties, density of states (DOS), charge mobilities, dipole moment, global reactivity descriptors, molecular electrostatic potential (MEP), transition density matrix (TDM), and OPV device-related parameters. The results revealed significant potential of the designed molecules as FREAs for OPVs, thus highlighting their suitability for further experimental exploration.
#### NIT-7

# Transition Metalides Based on Facially Polarized All-Cis-1,2,3,4,5,6-Hexafluorocyclohexane – A New Class Of High Performance Second Order Nonlinear Optical Materials

## Dr. Khurshid Ayub

#### Department of Chemistry, COMSATS University, Abbottabad, KPK, Pakistan

Abstract: Continuous attempts are being made to discover new approaches to design materials with extraordinary nonlinear optical response. Herein for the first time, we report the geometric, electronic, and nonlinear optical properties of novel Janus transition metalides AM-J-TM (where AM =Li, Na, K, TM = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn) containing alkali metals as source of excess electrons for transition metals to generate metalides. The Janus organic complexant used for the study is all cis 1,2,3,4,5,6-hexafluorocyclohexane F6C6H6 (J). These complexes contain unique involvement of alkali metals (AM = Li, Na, K) as source of excess electron which significantly affects the hyperpolarizability values of the resulting transition metalides. The NBO analysis reveals the charge transfer from alkali metals to the transition metals thereby confirming the metalide behavior of complexes. Moreover, the metalide nature of these complexes is validated through frontier molecular orbital (FMO) analysis. The values of interaction energies, vertical ionization potential (VIP) and vertical electron affinity (VEA) illustrate the stability of metalide complexes. Ultimately, the hyperpolarizability values confirms the excellent nonlinear optical response of the designed transition metalides. The remarkable static first hyperpolarizability ( $\beta$ o) response up to 4×108 is observed for complexes of vanadium . Similarly, the complexes of AM-J-Mn and Li/Na-J-Sc show significantly high NLO response. These compounds besides providing a new entry into excess electron compounds will also pave the path for designing and synthesis of further novel NLO materials

# Eco-Friendly Nanocomposite Membranes for Removal of Heavy Metals and Biofouling from Industrial Effluents

Dr. Farha Masood

COMSATS University, Islamabad

Presenting Author: Dr. Farha Masood

Abstract: The global scarcity of clean water is a serious challenge to the survival of all living organisms. Membrane technology represents a promising solution to solve this critical issue. In this study, nanocomposites were developed by incorporating copper (Cu) nanoparticles on sepiolite (SP) through a chemical reduction method. The copper-loaded sepiolite (Cu/SP) was characterized by various microscopy and spectroscopy techniques. Subsequently, Cu/SP was added into a polyvinyl alcohol (PVA) matrix to develop Cu/SP@PVA nanocomposite membranes. The mechanical properties of the Cu/SP@PVA nanocomposites were significantly enhanced as compared to pure PVA membranes. Physical properties of nanocomposite membranes were investigated. Batch adsorption experiments were conducted to evaluate the adsorption capacity of Cu/SP@PVA nanocomposites for removal of chromium and lead from the industrial effluents. The effects of initial pH, adsorbent dosage, contact time, different types of heavy metal ions, and initial heavy metal ion concentrations on the adsorption capacity of the Cu/SP@PVA nanocomposites were investigated. The Cu/SP@PVA nanocomposite membranes depicted excellent chromium and lead removal properties. Moreover, the Cu/SP@PVA nanocomposite membranes exhibited strong antibacterial activity in simulated contaminated wastewater. In conclusion, Cu/SP@PVA nanocomposite membranes could be a promising candidate for the treatment of industrial effluents for the removal of heavy metals and biofouling.

## **OT1**

# Soft Lithographic Surface Patterning of in-situ PEG Nanocomposite Hydrogels for Selective Interface Interaction

Dr. Mehwash Zia

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## Presenting Author: Dr. Mehwash Zia

**Abstract:** The successful development of novel biomaterials requires understanding of protein adsorption and cell adhesion on engineered surfaces. The physically mixed and chemically synthesized poly(ethyleneglycol)-hydroxyapatite (PEG nHAp) based nanocomposite hydrogels were examined for the main influential factors of chemistry, topography and elasticity. The chemical and morphological structure of poly(ethyleneglycol)-hydroxyapatite (PEG nHAp) nanocomposite hydrogels was investigated via electron microscopy, X-ray diffraction (XRD) and spectroscopic methods (FTIR, RAMAN). Unique chemical and mechanical micro patterns were fabricated by Fill molding In Capillaries (FIMIC). To study the impact of hydroxyapatite on cell adhesion and protein adsorption FIMIC patterns were tuned so as to exhibit no topography in the hydrated state. A pronounced level of differential protein adsorption and homogeneous hydroxyapatite deposition from simulated body fluid (SBF) possessing distinct interfaces could be observed for chemically synthesized PEG nHAp hydrogel composites. Ultimately, cell adhesion experiments were performed, in which the cell adhesion behavior of osteoblasts and fibroblasts were observed on Poly(ethylene glycol)-Hydroxyapatite nanocomposite hydrogels.

## **OT2**

## ОТ3

# Evaluation of the Therapeutic Potential of Nano-Coated Drugs in In-Vitro and In-Vivo Models in Brain Cancer

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## Presenting Author: Dr Aneela Javed

Abstract: Glioblastoma multiforme (GBM), a highly aggressive grade IV brain tumor, has a poor prognosis with a median survival of only 15 months post-treatment and resistance to standard therapies like Temozolomide (TMZ). The retinoblastoma protein (pRB) pathway, a key genetic driver of GBM, offers a promising therapeutic target. To overcome the limitations of conventional treatments, natural compounds with anti-cancer, anti-inflammatory, and antiproliferative properties were explored. Various compounds were tested naked as well as their nano formulations using in vitro cell culture models of cell lines. All those formulations, that showed promising results in vitro were further tested on orthotopic xenograft mouse models of brain cancer. Promising results of enhanced targeted delivery of gfp labelled DNA was observed in chitosan coated nano formulations compared to non capsulated formulations, both in vitro and in vivo. Varius drugs encapsulated in stearic acid solid lipid nanoparticles (SLNP-S) and chitosan nanoparticles showed promising results of enhanced bioavailability, better blood-brain barrier penetration, and reduce toxicity. Physico-chemical characterization confirmed the stability, size, and controlled drug release of SLNP-S. In vitro assays on GBM cell lines (U87, U251) and non-cancerous HEK-293 cells demonstrated a dose- and timedependent reduction in cancer cell viability, while exhibiting minimal cytotoxicity in HEK-293. These formulations significantly inhibited cancer cell migration, indicating strong antimetastatic potential. These findings underscore the potential of silymarin and diosgenin nanoformulations as effective dual-targeting agents for GBM and cancer-induced inflammation, warranting further in vivo validation in orthotopic xenograft models.

# Enhanced Heat Transfer of Minichannel Heat Sink With Graphene Based Nanofluids

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## Presenting Author: Dr. Asif Khan

Abstract: The rapid advancement in new electronic systems has led to excessive heat dissipation. Recently, mini/microchannel heat sinks and nanofluids have emerged as viable options for properly dissipating excessively generated heat. However, the combination of small channel sizes and nanofluids results in a significant drop in flow pressure within the minichannel heat sinks, thereby restricting their further applications. GNPs nanofluids have recently demonstrated the potential to lower pressure drop and enhance heat dissipation phenomena. Thermal and hydrothermal performance of pin fin heat sink with graphene nanoplatelets nanofluids in comparison to distilled water has been investigated in a minichannel heat sink Water based GNPs nanofluids was used having concentration of 0.01% and Re in the range of 530 to 1237. Square pin fin with 1 mm depth, 1 mm width are analysed to a bottom heated surface of rectangular minichannel. For various heating power, the effect of Re and volumetric flow rate on the Nu, heat transfer coefficient, wall temperature, thermal resistance, pressure drop, pumping power, and friction factor are analysed. Experimentation was carried out at heating powers of 40W. Higher pumping power was observed for graphene nanoplatelets (GNPs) at all higher heating in comparison to distilled water. Thermal performance of GNPs nanofluids decreases with increasing heating powers. Maximum heat transfer enhancement and lowest base temperature for GNPs nanofluids were found to be 20.64% and 2.85% respectively at Reynolds number of 1237. Flow rate and heat flux were found responsible for pumping power.

# Demonstrating Donor-Acceptor Covalent Conjugate Of Polythiophene and Perylene Diimide as an All Organic Photocatalyst For Enhanced Light-Driven H<sub>2</sub>O<sub>2</sub> Production

Sana Iqbal‡, Faseeh Akbar‡, Muhammad Ahsan Salar, Tahir Sajjad Butt, Ammar Ahmed Khan, Manzar Sohail and Basit Yameen\*

Lahore University of Management Sciences, LUMS

Presenting Author: Sana Iqbal

Abstract: Photocatalytic production of hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) is being extensively explored as a cleaner route to one of the most consumed oxidants. In this context, precisely designed organic semiconductor polymers have only recently been recognized as promising photocatalysts. Contributing to this emerging area, herein, we present the potential of a donoracceptor covalent conjugate of polythiophene (PTh) and perylene diimide (PDI) as an allorganic photocatalyst for the artificial photosynthesis of H<sub>2</sub>O<sub>2</sub>. Such donor-acceptor conjugates of organic semiconducting polymers are referred to as double cable polymers (DCPs). The DCP employed in this study PTh-PDI-DCP is derived from the covalent conjugation of electron donor polythiophene and acceptor pervlene diimide (PDI). Compared to the individual components P3HT, PDI and their physical hybrid (P3HT-PDI-PH), the PTh-PDI-DCP exhibited superior fluorescence and (photo)electrochemical characteristics. All the photocatalysts were supported on a porous PVDF membrane for their convenient application as photocatalysts over multiple cycles. A comparison of the photocatalytic H<sub>2</sub>O<sub>2</sub> production rates averaged over 7 photocatalytic cycles suggests that the PTh-PDI-DCP photocatalyst is respectively 1.56, 2.43, and 1.35 times more active than the P3HT, PDI and P3HT-PDI-PH. Furthermore, the H<sub>2</sub>O<sub>2</sub> production using DCP photocatalyst has significant contributions of 2eone-step oxygen reduction reaction (ORR) and water oxidation reaction (WOR). Overall, this work reveals for the first time the photocatalyst potential of all organic DCPs for the photocatalytic production of H<sub>2</sub>O<sub>2</sub>.

## Amino Acid Functionalized Co-BTC MOF as an Efficient Electrocatalyst for OER

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Presenting Author: Khalid Talha

**Abstract:** The Chiral-Induced Spin Selectivity (CISS) effect can be used to improve the efficiency of OER by spin-filtering the anodic current. The CoBTC MOF modified with L-glutamine and DL-glutamine (CoBTC-G, CoBTC-DL) were characterized by XRD, Raman, FTIR, elemental analysis, SEM, TEM and it was confirmed that the MOFs have successfully been modified with amino acid. Pristine and modified MOFs were used as a catalyst to modify electrode for OER. The maximum current density achieved by CoBTC-G is 74.17 mA cm<sup>-2</sup> at 1.99 (V vs RHE), while 69.34 mA cm<sup>-2</sup>, 50.05 mA cm<sup>-2</sup> was achieved by pristine CoBTC and CoBTC-D (modified with DL-glutamine) respectively. The CoBTC, CoBTC-G and CoBTC-DL achieved current density of 10 mA cm<sup>-2</sup> at over potential of 384 mV, 392 mV and 424 mV respectively. The tafel slope values calculated for the CoBTC, CoBTC-G and CoBTC-DL are 189, 170 and 234 mV/sec respectively which shows that the reaction rate of the CoBTC-G is faster than the other two materials. The stability of the MOFs was analysed by Chronoamperometry at current density of 10 mV cm<sup>-2</sup> for 24 hrs.

# Development of PLCL/Chitosan Nanofibrous Membranes Loaded with Nicotinamide and ZnO-NPs of Ocimum Basilicum For Wound Repair and Skin Regeneration

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#### Presenting Author: Ghulam Murtaza Khuhro

**Abstract:** Nanofibrous materials have emerged as key players in skin regeneration therapy. This study investigates the synthesis of PLCL/Chitosan based nanofibrous membranes loaded with nicotinamide and ZnO-NPs of Ocimum basilicum, aimed at promoting rapid wound healing and preventing scar formation. To evaluate their effectiveness, both in vitro and in vivo assessments were conducted to examine the physicochemical and biological properties of the newly synthesized nanofibrous membranes. ZnO-NPs showed a fine, spherical shape with a multi-faceted structure with uniformly sized. ZnO-NPs had optical band gaps of 3.395 eV, and their zeta potential in distilled deionized water was measured at  $-23.3 \pm 0.713$  mV, indicating a strongly anionic nature. The DPPH (2, 2-diphenyl-1-picrylhydrazyl) assay for the antioxidant activity of ZnO-NPs has shown the highest antioxidant activity (97.8 %) as compared to plant extract (80.9 %). While in vitro cell viability was tested by using NIH 3T3 mouse fibroblast cell lines (5 × 104 cells/well). Cell viability of PLCL/Chitosan/Nicotinamide/ZnO-NPs was noted at 97.3 %, which confirmed that the material becomes good for the cell environment, also helpful in cell growth. Further, the in vivo assessment of the open wound of rats fully recovered, 100 % wound closure within 12 days showed collagen deposition and high vascularization in the cytohistological assay. In the light of above results, the present material demonstrated notable antimicrobial, antioxidant, and skin regenerative properties, positioning it as a promising candidate for advanced wound dressings and drug delivery systems, thereby greatly enhancing the wound healing process.

# Comparative Analysis and Green Synthesis of SWCNTs and MWCNTs Electrodes Modified with MOF (ZIF-67) and Laser-Ablated Ag Nanoparticles for Electrochemical Detection of Glucose.

Ramsha Taffazul<sup>1</sup>, Ayesha Noor<sup>2</sup>, Peer Muhammad<sup>1</sup>, Hamza Qayyum<sup>2</sup>, Sana Ghaffar<sup>1</sup>, Sofia Javed<sup>1</sup>, Muhammad Irfan<sup>1</sup>

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#### Presenting Author: Ramsha Taffazul

Abstract: Diabetes is a prevalent health condition across the globe, impacting millions of patients and posing serious complications if not controlled in a proper manner. Glucose monitoring is of paramount importance in managing diabetes, and electrochemical sensors have been found to be a promising method of glucose detection in real-time. Among these, carbon nanotubes, i.e., multi-walled carbon nanotubes (MWCNTs) and single-walled carbon nanotubes (SWCNTs), have been of immense interest due to their remarkable electrochemical properties. In this comparative analysis, the electrochemical response of MWCNTs and SWCNTs in glucose detection is compared in terms of their sensitivity, limit of detection (LOD), and impact of modifying these materials using silver (Ag) and metal-organic frameworks (MOFs) using a green synthesis approach. Various characterization techniques including Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), and Raman spectroscopy were employed to ascertain structure, chemical, and morphological properties of the nanotubes and their modified counterparts. The surface morphology was viewed in detail via SEM, while their crystallinity was confirmed via XRD. FTIR and Raman spectroscopy was employed to determine functional groups and to investigate interactions between glucose molecules and the nanomaterials. The incorporation of Ag and MOF in MWCNTs and SWCNTs via a green synthesis process highly enhanced the electrochemical response of the sensors. The Ag and MOF-modified MWCNT and SWCNT sensors displayed higher sensitivity and a lower LOD, of which the sensor based on SWCNTs displayed better results having sensitivity 15.5 mA/mM/c [m] ^2 and LOD 0.016946mM (S/N=3) & the Ag modified SWCNT electrode showing sensitivity= 17.56 mA/mM/c [m] <sup>^</sup>2 and LOD: 0.00674 mM. The work shows that green-synthesized Ag and MOF-added CNTs hold great potential to enhance glucose detection sensors for diabetic control, providing a green and efficient path to sensor design.

# "Revolutionizing the Domains of Restorative Dentistry"; Clinical Efficacy of Novel Nano-reinforced Dental Adhesives in Reducing Post-operative Sensitivity in Composites : A Randomized Clinical Trial

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#### Presenting Author: Nehal Amir

Abstract: Background Nanotechnology is the pivot of contemporary dental practice. By embodying dental biomaterials with nanoparticles, it has transfigured the domains of clinical dentistry. Post-operative sensitivity in composite restorations can be resolved by incorporating nanoparticles in dental adhesives. Objective To evaluate the effectiveness of a novel titaniananoparticle reinforced dental adhesive on post-operative sensitivity in composites. Methodology This triple-blinded, randomized clinical trial was conducted at the department of Operative Dentistry and Endodontics, School of Dentistry, Islamabad. A total of participants (n = 60) having Class- I and II cavitations with a minimum cavity depth of 3mm were included in the trial. They were randomly assigned into two groups A and B (n = 30). After informed consent, restorative intervention was accomplished using an etch-and-rinse adhesive strategy. In Group A, titania-nanoparticle-incorporated dental adhesive was used for composite restoration, while in Group B, adhesive without nanoparticles was employed. The primary outcome "Post-operative sensitivity" was assessed using Visual Analogue Scale (VAS) mean score. Participants were instructed to rate their sensitivity status at follow-up periods: 24 hours, one week, and one month. Mann-Whitney U test was employed to compare sensitivity between the two groups. Results According to results of this trial, a significant difference was observed between the two groups after 24 hours (p = 0.004) and one week (p = 0.002). However, no discernible difference was observed after one month (p = 0.643). Conclusion The incidence and severity of post-operative sensitivity is significantly lessened utilizing titania nanoreinforced adhesives as compared to conventional adhesives without nanoparticles.

## Impact of Computational Advancements on the Design of 2D-Materials

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## Presenting Author: Syed Atta Hussain

Abstract: Advancements in computational power and algorithms at a breathtaking speed can be frightening as well as a great engineering tool for designing and tailoring two-dimensional (2D) materials. These materials including graphene, transition metal dichalcogenides (TMDs), hexagonal boron nitride (h-BN), etc., possess extraordinary mechanical, electronic, and optical properties, making them the best candidates for applications in nanoelectronics, energy storage, and quantum computing. Computational techniques play an important role in designing and tailoring the properties of 2D materials. Using density functional theory (DFT) electronic structure can be determined and for mechanical and thermal properties molecular dynamics (MD) can be utilized. For designing and optimizing new stable configurations of 2D materials AI and machine learning methods can be implemented. This article focuses on the importance of computational advancements in designing and predicting the properties of 2D materials. We will go through the impact of the discovery of 2D materials on wider materials research and how computational techniques aid these advancements. Available computational methods for 2D materials will also be discussed along with their background and advancing trends. We will also compare the current computational techniques for specific applications. Case studies will also be discussed along with limitations and challenges for computational techniques. In the end, we will present some future recommendations for interdisciplinary collaboration of materials science and computational sciences for sustainable engineering and innovations in nanotechnology.

# Design and Analysis of a Supramolecular Gel Electrolyte With Enhanced Mobility for Li-Ion Batteries

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## Presenting Author: Farooq Ahmad

Abstract: Supramolecular gel electrolytes (SGEs) are vital for Li-ion batteries, offering enhanced ionic conductivity, improved safety, and higher stability for advanced energy storage. Here, we present the fabrication of an SGE composed of lithium tetrafluoroborate (LiBF4) salt dissolved in propylene carbonate (PC) with the addition of a gelator (G2). The SGE was formulated with a concentration of 1M LiBF4, with a gelator conc. of 20%. To characterize new type of solid electrolyte for Li-ion based systems we have used optical spectroscopy methods (FTIR and Raman), nuclear magnetic resonance methods (NMR spectroscopy and diffusometry), dielectric spectroscopy (DS), thermal analysis (TGA/DSC), and scanning fluorescence confocal microscopy (SFCM). Obtained results concerns inter- and intramolecular interactions in both the pure solvent and the gel electrolyte sample, ionic conductivity of liquid electrolyte and SGE, translational dynamics of solvent molecules and dissociated ions, determination of the transference number, phase transition and thermal stability determination, and characterization of the internal matrix microstructure. Experiments performed as a function of temperature allowed us to determine the application potential of designed materials as supramolecular electrolytes for Li-ion based energy devices. The good thermal stability, high translational dynamics, well-defined internal microstructure and low burden on natural environment allows to think about these systems as future successors of conventional polymer gel electrolytes.

# Numerical Insights into High-Indium InGaN NIR LEDs: A Path to Efficient Nano-Optoelectronics

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## Presenting Author: Iqra Anjum

Abstract: Near-infrared (NIR) InGaN light-emitting diodes (LEDs) with varying indium content are numerically investigated to explore their potential in nanofabrication and nanooptoelectronic applications.. InGaN based high-indium infrared LEDs are rarely explored due to severe charge localization, reduced carrier wavefunction overlap, and diminished internal quantum efficiency (IQE), ultimately leading to poor device performance. In this study, we propose a high indium content NIR LED and analyze its optoelectronic characteristics. The investigation considers indium compositions ranging from 49% to 65%, revealing a redshift in emission and broadening of the full width at half maximum (FWHM) with increasing In concentration. Notably, increase in the peak IQE with a minimized IQE droop is observed as In content was increased. Moreover, this study reports an optimized In content device which reduces the quantum confined Stark effect in the active region thereby improving the electron and hole wavefunctions overlap. This design modification significantly enhances carrier recombination efficiency. As a result, the proposed LED demonstrates an IOE of  $\sim 80\%$ , surpassing the previously reported 70%, along with a notable improvement in output power. These findings emphasize the potential of InGaN-based nanostructured LEDs for advanced NIR nano-optoelectronic applications, contributing to the development of next-generation nanodevices.

## Formulation of Herbal Nano-sponge for Diabetes Treatment

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Presenting Author: Sana Saleem

Abstract: Diabetes mellitus remains a significant global health concern, with conventional treatments primarily focused on restoring beta-cell function through pharmacological interventions. Despite these efforts, effective management of hyperglycemia continues to pose a major challenge. In recent years, nanosponge technology has emerged as a promising strategy for targeted glucose removal from the bloodstream. The use of biocompatible, food-derived components in nanosponge formulations offers a promising approach to achieving safe and effective glycemic control, reducing the potential for adverse effects while enhancing therapeutic efficacy. This study explores the potential of basil seed mucilage for formulating glucomannan-based nanosponges aimed at managing hyperglycemia. The physical and chemical properties of the glucomannan nanosponges were characterized using UV, FTIR, and XRD while particle size and charge were assessed using DLS and Zeta analysis. FESEM analysis revealed an interconnected porous structure with particle size distribution centered around 25nm. Solubility and stability studies were conducted in simulated body fluids, including SBF (pH 7.4), SGF (pH 1.2), and SIF (pH 6.8). The nanosponges showed good solubility in SGF and exhibited stability for up to 24 hours before degradation, indicating their potential to transit through the gastrointestinal tract without agglomeration. In simulated intestinal fluid (SIF), the nanosponges remained stable for up to 38 hours, suggesting they could absorb glucose effectively in the intestine, where most digestion occurs. A glucose absorption study demonstrated an increase in sugar absorption over time. In vitro cytotoxicity studies, using NIH3T3 mouse fibroblast cells, confirmed the biocompatibility and non-toxic nature of the glucomannan nanosponges.

## **Quercetin-Loaded Nano Formulation for Diabetes Management**

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## Presenting Author: Asma Jaffer

Abstract: Diabetes mellitus (DM) is a prevalent metabolic disorder characterized by chronic hyperglycemia due to impaired insulin secretion or function, leading to severe complications affecting both microvascular and macrovascular systems. Despite the availability of insulin and oral hypoglycemics agents, their limitations necessitate the exploration of alternative therapeutic strategies. Phyto-derived bioactive compounds, such as quercetin, exhibit significant antidiabetic potential by promoting  $\beta$ -cell regeneration and enhancing insulin secretion. However, their clinical application is hindered by poor bioavailability, rapid degradation and premature release. To address these challenges, we developed a quercetinloaded nano formulation using dietary fiber arabinoxylan extracted from flaxseed as a biopolymer matrix. Nanoparticles were synthesized via the solvent evaporation method and characterized using FT-IR, XRD, FESEM, DLS and zeta potential analysis. Nanoformulations offer numerous advantages, including high drug loading capacity, sustained release, improved bioavailability and targeted accumulation in diabetic tissues, thereby enhancing therapeutic efficacy while minimizing side effects. This study underscores the potential of nanomedicine in revolutionizing phytonutrient-based diabetes management by ensuring controlled and efficient drug delivery.

# Fabrication of pRNA Nanoparticles for Targeted Regression of MYCN Gene Overexpressing Human Cancers

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Presenting Author: Asima Asghar

**Abstract:** Background: The MYCN oncogene is a key driver of aggressive cancers like neuroblastoma and small cell lung cancer. Targeted therapies are essential for treating such cancers. This study presents the fabrication of aptamer-functionalized pRNA nanoparticles co-assembled with MYCN-specific siRNA and CY5.5 for targeted gene silencing.

Objectives: 1. Synthesis and characterization of pRNA nanoparticles with aptamers, siRNA, and CY5.5. 2. Overcoming resistance mechanisms in MYCN-amplified cancers. 3. Evaluation of the efficacy of RNA nanoparticles in suppressing tumor growth in MYCN-amplified cancer cell lines. Methods and Results: pRNA nanoparticles were synthesized and assembled in-house, validated through gel electrophoresis, and dynamic light scattering. In MYCN-amplified IMR-32 neuroblastoma cells, these nanoparticles showed efficient binding, internalization (confirmed via confocal microscopy), and reduced cell viability by 58% (MTT assay) compared to scrambled siRNA controls. TUNEL assays confirmed apoptosis, and RT-PCR revealed reduction in MYCN mRNA expression. Conclusion: This RNA-based therapy shows significant promise for cancer treatment. These pRNA nanoparticles have demonstrated efficacy in preclinical studies, positioning them for potential clinical trials to assess their role in targeted cancer therapies in Pakistan.

# The Rational Design of Green Nanocomposites Materials for Environmental Detoxification of Pollutants

## Rooh Ullah

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## Presenting Author: Rooh Ullah

Abstract: The sulfur adsorption capacity of the adsorbents strongly depends on the pore structure, the chemical states and the dispersion of active species. In this work, ZnO-Al2O3 mixed oxides with an improved structure were synthesized via a freeze-drying modified cation-anion double hydrolysis (CADH) technique and used as the support. Freeze drying technique provided the adsorbent with a smaller sized ZnO and an improved pore structure compared with the normal oven drying method. Micro fibre alumina was synthesized using thermal urea precipitation technique and applied as support for the nano-sized ZnO precursor. The facile functionalization of nano sized ZnO in reactive adsorption desulfurization (RADS) performance and effect of diffusion rate in the desulfurization process were compared with commercially prepared alumina used as support for ZnO and Ni precursors. Higher breakthrough desulfurization activity and sulfur adsorption capacity were concluded that strongly depends on the diffusion rate of molecules, homogenous nano-sized ZnO dispersion and degree of active oxides interaction with support. Detailed characterization results conclude that higher external diffusion of reactant molecules within the cress crass micro-fibre, nanosized ZnO particles and their lower irreversible oxides interactions (IOI) may be the reasons for superior RADS performance of Ni/ZnO-Al2O3-fibre adsorbent.

# Multi-Phase Transfer Studies of Diverse Iron Oxide Nanoparticles: Characterization and Insights

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## Presenting Author: Haroon Zafar

Abstract: Iron oxide nanoparticles (IONPs) have garnered significant attention in biomedicine owing to their unique magnetic properties and biocompatibility. However, achieving monodisperse nanoparticles with precise size control remains challenging. In this study, we investigated six thermal decomposition synthesis methods employing three iron precursors: iron oleate, iron pentacarbonyl, and iron acetylacetonate, to understand their effects on nanoparticle morphology, crystallinity, and magnetic properties. Characterization of the synthesized nanoparticles was performed using a combination of techniques including x-ray diffraction (XRD), Transmission Electron Microscopy (TEM), Vibrating Sample Magnetometer (VSM), and Microwave plasma atomic emission spectrometry (MP-AES). Results reveal that IONPs synthesized using iron pentacarbonyl exhibit the least crystallinity and magnetization, featuring a core-shell structure, while those synthesized with iron oleate and iron acetylacetonate display crystalline properties, with superior magnetization observed in the iron acetylacetonate-derived particles. Subsequently, various phase transfer methods, including KOH-assisted phase transfer, oxidative cleavage, and ligand exchange, were explored. Oxidative cleavage using KMnO<sub>4</sub> emerged as the most suitable method, preserving the physicochemical properties of IONPs. Following oxidative cleavage, KOH-assisted phase transfer and ligand exchange methods were ranked based on their minimal alteration of physicochemical properties and ease of implementation.

## **Electrospinning: A Revolution in Tissue Engineering**

# Saba Zahid, Ushan Hussain, Hafiza Sunaina Aijaz, Hafsa Akhtar, Ather Farooq Khan, Hamad Khalid

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## Presenting Author: Hamad Khalid

Abstract: Electrospinning has emerged as a revolutionary technique in tissue engineering due to its ability to create nanofibrous scaffolds that mimic the extracellular matrix (ECM) of tissues. The unique properties of these scaffolds such as their high surface area, porosity, and versatility in material selection make electrospinning a powerful tool for developing artificial tissues and organs. With the growing demand for skin regeneration products, materials promoting wound healing are being developed. Antioxidants, such as vitamin E (VE), play a key role in inflammation, cell proliferation, and remodeling during wound healing. A bi-layered electrospun membrane with a lower polycaprolactone (PCL) layer and an upper polylactic acid (PLA) layer, loaded with VE, was created and evaluated. SEM images showed fiber diameters of 1-6 µm, with VE affecting fiber morphology. These membranes' porous, biocompatible structure makes them promising for skin regeneration and wound healing. Similarly, for effective bone regeneration, tissue-engineered scaffolds must resemble bone and possess properties like biocompatibility, biodegradability, osteogenic, osteoconductive, and osteointegrative capabilities. Fabrication of core-shell ultrafine fibers using electrospinning, with Polycaprolactone (PCL) as the inner layer, hydroxyapatite encapsulated within it, and a PLA outer shell containing zinc oxide (ZnO) for its antibacterial properties. The electrospun membranes display antimicrobial activity due to the presence of ZnO. In the continuation of bone regeneration, we developed tri-layered composite nanofibrous membranes designed to mimic the bone extracellular matrix (ECM) for bone tissue regeneration. The outer layer, made of poly(lactic acid) (PLA) infused with Zr-ZnO nanoparticles, provides antibacterial properties. The middle layer, consisting of poly(caprolactone) (PCL) and Vitamin E, supports osteoblast activity, while the inner layer, composed of silk fibroin (SF) and silicon-doped hydroxyapatite (Si-HA), offers mechanical strength and calcium phosphate for bone regeneration. Overall, the tri-layered scaffold showed great potential for bone tissue regeneration by enhancing mineralization, cell attachment, and proliferation.

# Dynamic Light Scattering Based Optimization Of Zinc Cobalt Sulfide Nanoparticles With Enhanced Energy And Power Density For Supercapictors Application

Hafeez Ur Rehman, Ahson Jabbar Shaikh

Comsats University Islamabad, Abbottabad Campus

Presenting Author: Hafeez Ur Rehman

Abstract: Zinc cobalt sulfide (Zn-Co-S) nanoparticles have gained attention as promising electrode materials for supercapacitors due to their outstanding electrochemical properties. However, achieving both high energy density and power density remains a challenge due to particle agglomeration and instability. In this study, dynamic light scattering (DLS) was employed to optimize the synthesis of Zn-Co-S nanoparticles by carefully adjusting key parameters such as temperature, pH, precursor addition rate, and stabilizer concentration. This approach led to the formation of smaller, more stable nanoparticles. The optimized Zn-Co-S electrodes exhibited an impressive specific capacitance of 1156 F/g, an energy density of 194 Wh/kg, and a power density of 7260 W/kg, which surpass previously reported values. Electrochemical impedance spectroscopy (EIS) analysis revealed a lower charge transfer resistance of 35.88  $\Omega$ , indicating improved ion transport and enhanced conductivity. Furthermore, the optimized electrodes demonstrated excellent cyclic stability, retaining 93.87% of their capacitance after 10,000 charge-discharge cycles. These findings emphasize the importance of nanoparticle size control in enhancing electrochemical performance and establish DLS-optimized Zn-Co-S as a highly efficient material for next-generation supercapacito

# Green Synthesis of Biocompatible Core-Shell (Au-Ag) and Hybrid (Au-ZnO and Ag-ZnO) Bimetallic Nanoparticles and Evaluation of their Potential Antibacterial, Antidiabetic, Antiglycation and Anticancer Activities

Khadija Nawaz, Bushra Ahmad, Christophe Hano, Bilal Haider Abbasi and Sumaira Anjum

## Kinnaird College for Women University, Lahore

Presenting Author: Dr. Sumaira Anjum

Abstract: The fabrication of bimetallic nanoparticles (BNPs) using plant extracts is applauded since it is an environmentally and biologically safe method. In this research, Manilkara zapota leave extract was utilized to bioreduce metal ions for the production of therapeutically important core-shell Au-Ag and hybrid (Au-ZnO and Ag-ZnO) BNPs. The phytochemical profiling of leave extract in terms of total phenolic and flavonoid content attributed to highest free radical scavenging activity. FTIR data also supported the involvement of these phytochemicals (polyphenols, flavonoids, aromatic compounds and alkynes) in the synthesis of BNPs. Whereas, TEM and XRD showed the formation of small sized (16.57 nm) spherical shaped core-shell Au-Ag BNPs and ZnO nano-needle with spherical AuNPs (48.32 nm) and ZnO nano-rod with spherical AgNPs (19.64 nm) hybrid BNPs. The biological activities of BNPs reinforced the fact that they show enhanced therapeutic efficacy as compared to their monometallic components. All BNPs showed comparable antibacterial activities as compared to standard tetracycline discs. While small sized Au-Ag BNPs were most effective in killing human hepato-cellular carcinoma cells (HepG2) in terms of lowest cell viability, highest intracellular ROS/RNS production, loss of mitochondrial membrane potential, induction of caspase-3 gene expression and enhanced caspase-3/7 activity. BNPs also effectively inhibited advanced glycation end products and carbohydrate digesting enzymes which can be used as nano-medicine for aging and diabetes. Most important findings were the permissible biocompatibility of these BNPs towards brine shrimp larvae and human RBCs which suggests their environmental and biological safety. This research study gives us an insight into the promise of using green route to synthesize commercially important BNPs with enhanced therapeutic efficacy as compared to conventional treatment options.

## CaO and MgO-Based Catalysts For the Synthesis of Drug Intermediates

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## Presenting Author: Shahzad Rasheed

Abstract: The efficient, selective, scalable, and sustainable synthesis of pharmaceutical intermediates is one of the vital elements of medicinal chemistry. We explored the thermoselective synthesis of dihydropyrimidinones (DHPMs) and 1,4-dihydropyridines (DHPs) via the Biginelli and Hantzsch reactions, respectively, in the presence of sulphonic acid functionalized mesoporous silica-coated magnesium oxide (MgO-SO<sub>3</sub>H) and calcium oxide (CaO-SO<sub>3</sub>H) as heterogeneous catalysts. The catalysts were prepared through the surface functionalization of CaO and MgO particles and characterized using FT-IR spectroscopy, XRD, SEM, and UV-Vis spectroscopy to determine their structural and acidic properties. The catalytic performance was evaluated under varying reaction conditions in a pressure tube, including temperature, reaction time, raw material ratios, solvent effects, catalyst loading, and recyclability. In all reactions, the highest product yields were achieved under solvent-free conditions. MgO-SO<sub>3</sub>H exhibited ~95% DHPM yield at 80°C, while CaO-SO<sub>3</sub>H gave ~74% DHPM yield. Above 100 °C, the reaction shifted to the Hantzsch pathway, leading to 98% DHP selectivity at 120 °C. The catalysts showed broad substrate applicability, efficiently converting aromatic and non-aromatic aldehydes and urea derivatives. Recyclability tests confirmed that MgO-SO<sub>3</sub>H remained stable over multiple reaction cycles. Mechanistic studies and GC-MS analysis provided insights into the intermediates governing DHPM and DHP selectivity. These findings offer an efficient, scalable, and sustainable approach for pharmaceutical intermediate synthesis.

# A New Green Switchable Dispersive Solid–Liquid Microextraction

## Using Multi-Walled Carbon Nanotubes For Selenium in Real Water Samples

## Presenting Author: Dr. Naeem Ullah

**Abstract:** Switchable hydrophobic-hydrophilic transition dispersive solid-liquid microextraction (SHT DSLME) was introduced to remove total selenium from water samples. Multiwalled carbon nanotubes treated with tetraethylenepentamine MWCNTs-TEPA were synthesised and used to remove and analyse total inorganic selenium using SHT-DSLME and graphite furnace atomic absorption spectrometry (GFAAS). This study achieved the hydrophobic-hydrophilic transition of MWCNTs-TEPA by exposing them to  $CO_2$ , a green, inexpensive, non-hazardous, and non-accumulating antisolvent trigger.

The hydrophobic-to-hydrophilic transition of functionalised MWCNTs was validated using FTIR and SEM studies. Maximised experimental conditions yielded 72 EF and 15.0 ug/L LOD for selenium. Validation of the developed method was carried out by selenium determination using water for trace elements as a certified reference material and the results were found to be in good agreement with the certified values. The new technology was successfully employed to measure selenium in real water samples.

# A Facile Synthesis of Co-Ni Nanoalloy Via Leidenfrost Effect For Fabrication of Robust Thin Films Having Enhanced EMI Shielding

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Fatima Jinnah Women University, Rawalpindi

Presenting Author: Qurat Ul Ain

**Abstract:** The synthesis of nanomaterials in a simple, efficient and environment friendly way is a promising pathway for the fabrication of lightweight and flexible electromagnetic interference shields. Transition metal nanostructures have become the centre of attention due to their versatile applications ranging from electronic to photonic devices. However, existing approaches for the synthesis of nanoparticles are either eco-unfriendly or challenging. The objective of this study was synthesis of Co-Ni nanoalloy and their fabrication with minimal environmental impact, having significant EMI shielding. Herein, we employed an innovative approach for the benign and economical synthesis of Co-Ni nanoalloy via "inverse-Leidenfrost effect." Synthesized nanoalloy were coated with carbon (CC-Co-Ni nanoalloy) and characterized through FTIR, XRD, SEM and TGA techniques. By applying the Scherrer's formula, the crystallite size of Co-Ni nanoalloy was calculated as 14.98 nm and CC-Ni-Co alloy as 18.17 nm. Co-Ni and CC-Co-Ni nanoalloy were further employed in the fabrication of free standing thin films via solvent evaporation technique with PVC matrix in varying concentrations. Thin films having novel architecture [Co-Ni@PVC] and [CC-Co-Ni@PVC] were successfully prepared and analyzed using Vector network analyzer, SEM, TGA and Tensile testing. Specifically, we aim to investigate the effect of filler concentration and their ratio with the polymer within the architecture [Co-Ni@PVC] and [CC-Co-Ni@PVC]. At the optimum ratio, the EMI shielding analysis of thin films having architecture [Co-Ni@PVC] and [CC-Co-Ni@PVC] showed appreciable shielding effectiveness of -28.86 dB and -42.86 dB, respectively. Furthermore, the [CC-Co-Ni@PVC] and [Co-Ni@PVC] thin films exhibited electrical conductivity of 1.67×10<sup>-5</sup> and 1.07×10<sup>-5</sup> S/cm, with significant mechanical stability, and thermal resistance as well.

# Silk Based Antibacterial-Osteogenic Composite Scaffolds for Simultaneous Regeneration of Soft and Hard Tissues

Saamia Naz, Hafsah Akhtar, Fahad Hussain Alhamoudi, Asma Tufail, Aqif Anwar Chaudhry, Muhammad Yar, Hamad Khalid\*, Ather Farooq Khan\*

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Presenting Author: Saamia Naz

Abstract: Barrier membranes are essential in guided bone regeneration (GBR), but their clinical use in orthopedic and dental applications is often limited by microbial contamination and the complexity of soft and hard tissue integration. To address these challenges, a novel nanocomposite sandwich-like GBR membrane (STEM) was developed using sequential electrospinning techniques. The membrane consists of silk fibroin, copper-doped bioactive glass (Cu-BG), and strontium-doped zinc oxide (Sr-ZnO), designed to enhance osteogenic activity and provide antimicrobial properties. Morphological analysis via Field Emission Scanning Electron Microscopy (FESEM) showed a reduction in fiber diameter with the addition of Sr-ZnO and Cu-BG. Surface wettability tests indicated improved hydrophilicity, favorable for cell adhesion. The membrane exhibited optimal swelling behavior, porosity, and surface roughness, all critical for supporting cell proliferation and attachment. Antibacterial assays confirmed activity against E. coli. Mechanical testing demonstrated a 2- to 6-fold increase in Young's modulus, indicating enhanced mechanical strength. In vitro degradation studies revealed approximately 80% degradation after 21 days, aligning with alveolar bone healing timelines (~28 days). Cell culture studies with MC3T3 cells showed 70-80% seeding efficiency and strong proliferation, confirming biocompatibility. Live/dead staining and migration assays indicated high cell viability and 98% wound closure within 24 hours. Alizarin red staining and calcium deposition assays confirmed enhanced mineralization. Overall, the STEM membrane shows strong potential for periodontal regeneration due to its bioactivity, biocompatibility, and osteogenic properties.

# Mg Doped ZnO Containing Silk Nanocomposite Scaffolds For Biofilm Prevention During Alveolar Bone Regeneration

Ayesha Shahid, Faisal Moeen, Sadia Habib, Aysha Arshad, Rabia Zeeshan, Aqif Anwar Chaudhry, Hamad Khalid, Fahad Hussain Alhamoudi, Hafsah Akhtar, Ather Farooq Khan

## COMSATS University Islamabad, Lahore Campus

#### Presenting Author: Sadia Habib

Abstract: Biofilms develop when micro-colonies adhere to a solid surface and produce a robust extracellular matrix, which increases the risk of infection and impedes the healing process of bone defects. Although postoperative antibiotics are often prescribed to prevent infections, they carry the risk of side effects and the potential for antibiotic resistance. Recent research has explored the use of magnesium-doped zinc oxide nanoparticles incorporated into silk fibroin scaffolds to hinder biofilm formation in applications related to alveolar bone regeneration. Innovative silk fibroin (SF)/hydroxyapatite (HA) scaffolds, embedded with magnesium-doped zinc oxide nanoparticles (Mg-ZnO NPs with 0.5%, 1% and 2% Mg), were fabricated using the freeze gelation method. The results indicated that these new materials exhibit notable antibacterial activity against Staphylococcus aureus. Moreover, these materials were also found to be biodegradable and biocompatible. The study revealed that the scaffolds displayed excellent antibacterial activity that increased with the concentration of Mg-doped ZnO nanoparticles, achieving a maximum effectiveness of 49.39% for the 2% Mg-doped ZnO. Additionally, biodegradation of the material also increased with higher concentrations of Mg doping in ZnO. The scaffolds demonstrated an adequate porosity level ranging from 67% to 74.3%, leading to improved cell viability (99.6%) and a uniform deposition of apatite on their surfaces, making them an excellent candidate for biomedical applications requiring antibacterial properties and high cell viability.

# Development of Halal Uni & Bi-functional Bioactive Scaffolds For Advanced Hard Tissue Repair

Maryam Aslam, Warda Aziz, Prof. Aqif Anwar, Prof. Ather Farooq Khan

## COMSTAS University Islamabad, Lahore Campus

## Presenting Author: Maryam Aslam

Abstract: The need for hard tissue repair and regeneration arises from disease, trauma, congenital defects, or aesthetic concerns. Traditional bone repair methods often use metal implants, autografts, allografts, xenografts, or synthetic bone grafts. Hydroxyapatite is widely used in bone regeneration, especially as bone fillers, where barrier membranes are employed to retain granules in place and protect the defect site from infection. Many existing products, including collagen-based guided tissue and bone regenerative membranes, are derived from non-Halal/porcine sources, raising ethical concerns for Muslim consumers. These products are also expensive and often inaccessible to the general population in Pakistan. In response, we have developed Halal-compliant sodium alginate crosslinked collagen membranes and pure collagen membranes, extracted from bovine sources. Using an in vivo subcutaneous implantation model, we evaluated tissue responses, including cellular infiltration, vascularization, and degradation, at 14 and 28-day intervals. The results showed favorable wound healing properties for all membranes. The sodium alginate crosslinked collagen membrane demonstrated biocompatibility and stability up to 28 days post-implantation, making it a viable candidate for Guided Bone Regeneration (GBR) applications. This poster introduces our project, funded by the Higher Education Commission of Pakistan, aimed at developing Halal Uni & Bi-functional bioactive scaffolds for advanced hard tissue repair.

## Cerium Oxide and Silk Fibroin Doped PLA Scaffold to Bridge Tendon

Sidra Tul Muntaha, Hafsah Akhtar, Saamia Naz, Sadia Habib, Hamad Khalid, Ather Farooq Khan

Interdisciplinary Research Centre in Biomedical Materials, COMSATS University Islamabad, Lahore campus, Lahore, Pakistan

Presenting Author: Sidra Tul Muntaha,

Abstract: Tendon injuries are often painful and debilitating, with surgical treatments frequently leading to scar tissue formation, increasing the risk of re-injury or rupture and complicating recovery. Tissue engineering approaches offer promising alternatives by providing biomimetic scaffolds that support tissue regeneration. In this study, a composite nanofibrous scaffold composed of silk fibroin (SF), polylactic acid (PLA) and copper-doped cerium oxide was fabricated using electrospinning. This technique enables the production of scaffolds with controlled mechanical and elastic properties, which are essential for supporting newly forming tendon tissue. The study aimed to fabricate both random and aligned nanofibrous scaffolds to mimic the native structure of tendons. The synthesized scaffolds were systematically characterized using various analytical techniques. Fourier-transform infrared spectroscopy (FTIR) confirmed the presence of functional polymeric groups, while scanning electron microscopy (SEM) revealed fiber morphology and alignment, demonstrating a structural resemblance to natural tendon tissue. The scaffolds exhibited optimal hydrophilicity, swelling capacity, porosity and density, which facilitated cell proliferation and enhanced cellular attachment to host tissues. Additionally, in vitro degradation studies indicated a favorable degradation rate, aligning with the regeneration period of the tendon regeneration. The mechanical properties of dry and wet scaffolds were analyzed post-degradation. The tensile strength of the scaffolds was found to align with the native tendon strength, indicating their potential suitability for tendon tissue engineering applications. Overall, the results suggest that the developed composite scaffold holds significant potential as a biomaterial for tendon regeneration, providing an effective platform for improved healing outcomes.

## Synthesis of Whitlockite Based Bioinks For Bone Tissue Regeneration

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## Presenting Author: Sadaf Batool

Abstract: To address the challenges of custom-made bone scaffolds, 3D printing has been explored widely. In this work, a bioceramic-based bio-ink has been prepared for the fabrication of 3D bone scaffolds. The alginate-gelatin polymer composite was prepared by Schiff-base chemical reaction. To this composite whitlockite (WH) nanoparticles were incorporated as reinforcement and the effect of these bioceramics on rheology, printability, and crosslinking of polymers was studied. The composite ink was printed in a grid structure with up to four layers. The functional group crosslinking of the bioink was confirmed by Fourier transform infrared spectroscopy (FTIR) analysis. The mechanical strength of the bioinks was measured using a universal tensile testing machine (UTS) and in-vitro bioactivity was evaluated under simulated body fluids. The cross-linking and rheology study confirmed that the mechanical strength, flowability, and printability of the bioink have improved with the addition of WH nanoparticles. The biological analysis confirmed that prepared bioinks are cytocompatible and have facilitated cell adhesion and proliferation. The bioink also demonstrated excellent bioactivity in SBF and the bioactivity potential increased with an increase in WH concentration. The obtained results confirmed that prepared bio-ink can be used for printing multiple layered 3D constructs that can be utilized for in-vivo bone tissue regeneration applications.

# Designing the Poly-Lactic Acid Functionalized Polymer Organic Framework Scaffolds For Wound Healing

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Comsat University Islamabad, Lahore Campus

## Presenting Author: Laiba Tehreem

Abstract: Wound healing is a complex biological process that requires an optimal environment to promote tissue regeneration and prevent infections. In this study, we designed and fabricated poly-lactic acid (PLA) functionalized polymer organic framework (POF) scaffolds through electrospinning for enhanced wound healing applications. Polymer organic frameworks (POFs) have emerged as promising materials for biomedical applications due to their high porosity, tunable functionality, and biocompatibility. PLA, a biodegradable and biocompatible polymer provides mechanical stability and controlled degradation, while the POF structure ensures high surface area for cell attachment, nutrient exchange, and drug delivery. The incorporation of bioactive agents and antibacterial components within the POF matrix further enhances the healing process by reducing inflammation and preventing microbial infections. The fabricated electrospun scaffolds were analyzed using various characterization techniques. The electrospun scaffolds were structurally and chemically characterized using Fourier Transform Infrared Spectroscopy (FTIR) to confirm functional group interactions and successful incorporation of the POFs within the PLA matrix. Morphology and fiber alignment of synthesized scaffolds was confirmed by Scanning Electron Microscopy (SEM). Evaluation of hydrophilicity, swelling, porosity and density of the PLA/POF scaffold showed that results were in optimal range that hold promise for future clinical applications, facilitating cell proliferation and promoting cell attachment to host tissues. The findings suggest that PLA-functionalized POF scaffolds hold great potential as advanced biomaterials for next-generation wound care applications.

# Fabrication and Characterization of Tri-Layered Electrospun Membranes for Bone Regeneration

hafiza sunaina ijaz, maryam shafique, hafsah akhter , ather farooq khan, hamad khalid

interdiciplanry rechearch center in biomedical materials

Presenting Author: hafiza sunaina ijaz

Abstract: Multilayer nanofibrous scaffolds are gaining significant attention in the biomedical field, particularly as materials for tissue regeneration and drug delivery. In this study, we present a unique design of tri-layered composite nanofibrous membranes that mimic the extracellular matrix (ECM) of bone for bone tissue regeneration. The superficial layer, made of poly(lactic acid) (PLA), is infused with Zr-ZnO nanoparticles to impart antibacterial properties. The middle layer consists of poly(caprolactone) (PCL) and Vitamin E, which promote osteoblast activity. The inner layer is composed of silk fibroin and silicon-doped hydroxyapatite (Si-HA), providing mechanical strength and calcium phosphate essential for bone regeneration. We examined the membranes in terms of morphological characterization and physicochemical properties. Fourier-transform infrared (FTIR) spectroscopy confirmed the presence of functional groups and the successful incorporation of additives within the trilayered structure. Scanning electron microscopy (SEM) imaging revealed the nanofibrous morphology and uniform dispersion of the additives. Contact angle measurements indicated that the PLA+Zr-ZnO layer exhibited higher hydrophobicity compared to the silk fibroin+Si-HA layer. Physical studies, including degradation, swelling, porosity, and density assessments, showed optimal results that will facilitate cell proliferation and promote cell attachment to host cells. Antibacterial studies demonstrated the exceptional potential of Zr-ZnO nanoparticles. The mechanical strength of silk was assessed using dynamic mechanical analysis (DMA). Overall, the results indicate that the proposed biocompatible tri-layered scaffold holds great promise as a material for bone tissue regeneration applications, offering improved mineralization, enhanced cell attachment, and increased cell proliferation.

# Ammonia-free Soft urea-derived Nickel Cobalt Nitride/CNTs as Battery-Type Electrode for Asymmetric Supercapacitors

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## Presenting Author: Fatima Anees

Abstract: Efficient and sustainable energy storage devices are critical to addressing global energy demands. Supercapacitors, with their fast charge-discharge capabilities and long cycle life, bridge the energy-power gap between batteries and capacitors. Transition Metal Nitrides (TMNs) offer excellent redox properties and conductivity but face challenges in stability and the environmental impact of ammonia-based synthesis methods. This study presents an ammonia-free, urea-based synthesis of Nickel Cobalt Nitrides (NiCoN) integrated with Carbon Nanotubes (CNTs) as next-generation supercapacitor electrodes. Different compositions of nickel and cobalt-based nitrides were synthesized with CNTs. The successful synthesis of the materials was confirmed by using several types of morphological and structural characterization techniques, including XRD, SEM, and TEM. The electrochemical performance of the samples with different metallic ratios i.e. NiCoN(1:1)/CNTs, NiCoN(1:2)/CNTs, and NiCoN(2:1)/CNTs were tested in three-electrode system, where NiCoN(1:1)/CNTs showed the best performance, exhibiting a remarkable specific capacitance of 1146.5 F g<sup>-1</sup> at a current density of 0.5 A g-1. Its battery-like behavior was assessed using Dunn's method. Furthermore, an Asymmetric Supercapacitor (ASC) was assembled with NiCoN(1:1)/CNTs as positive and Activated Carbon (AC) as a negative electrode. The NiCoN(1:1)/CNTs // AC device achieved a high energy density of 79.7 Wh kg-1 and a power density of 243.75 W kg<sup>-1</sup> at 0.35 A g-1. Notably, the device retained 101.8 % capacity and maintained an overall coulombic efficiency of 98 % after 10,000 repeated cycles, demonstrating high cyclic reversibility.

# Cation-Intercalated Pillared Carbonitride (Ti<sub>3</sub>CNTx) MXenes for Superior Energy Storage Application

## Aiza Kanwal, Sheryar Abid, Syed Rizwan

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#### Presenting Author: Aiza Kanwal

**Abstract:** This study presents a comprehensive methodology for the etching and delamination of carbonitride (Ti<sub>3</sub>CNT<sub>x</sub>) MXenes, alongside protocols for the intercalation of alkali and alkaline earth metal ions (Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>, Mg<sup>2+</sup>) into these materials. Post-intercalation, the resulting composites exhibit exceptional performance as supercapacitor electrode materials, with K<sup>+</sup>-intercalated Ti<sub>3</sub>CNT<sub>x</sub> demonstrating an ultra-high capacitance of 1530 F g<sup>-1</sup> at a scan rate of 2 mV s<sup>-1</sup>. Moreover, the intercalation of cations enhances charge storage kinetics by extending charge/discharge times and reducing solution resistance and charge transfer impedance, indicative of improved ion transport pathways. Structural analysis reveals a significant increase in the c-lattice parameter and interlayer d-spacing, attributed to the effective accommodation of cations within the MXene framework. These findings underscore the potential of cation intercalation for tailoring MXene properties, offering a pathway for the design of advanced energy storage materials with remarkable electrochemical performance.

## Electrochemical Synthesis of Green Ammonia by Functionalized MXene (Ti3C2Tx)

# Asad Khalil

#### Lahore University of Management and Sciences

## Presenting Author: Asad Khalil

Abstract: The industrial process of ammonia synthesis, also called the Haber-Bosch (HB) process, requires high pressure (150-200 atm) and temperature (500°C). Moreover, in this process, CO<sub>2</sub> is released as a byproduct that causes global warming. Thus, the increasing demand for economical and eco-friendly nitrogenous fertilizers focusing on electrocatalytic nitrate reduction (eNitRR) into green ammonia (NH3) as a substitute for the Haber-Bosch (HB) process has gained significant scientific interest in the recent years. Nitrates are an industrial waste with severe health impacts that include methemoglobinosis, digestive system cancer, and blue baby syndrome; furthermore, it contributes to environmental issues like eutrophication, biodiversity loss, and greenhouse gas emissions. For e-NitRR, there are some challenges, such as high overpotential and low ammonia yield and selectivity; these problems highlight a potential research gap for finding highly efficient electrocatalysts. In the present study, the functionalized MXene, a class of two-dimensional materials having excellent electronic conductivity, tunable layer structure, and controllable interfacial chemistry, has been investigated for electrocatalytic application alongside the effect of different termination groups employed to functionalized MXene. The functionalized MXene is synthesized by etching an A layer from the parent molecule MAX (Ti<sub>3</sub>AlC<sub>2</sub>) phase into MXene(Ti<sub>3</sub>C2Tx) where Tx (OH, O, F, and Cl) is the termination group. In this study, we investigated faradic efficiency, yield and rate of ammonia production under different functionalization. Advanced characterization techniques, including FESEM, EDX, and XRD, were applied to elucidate the structural morphology, crystallinity, and phase analysis of functionalized MXene. The electrochemical analysis of the synthesized MXenes was performed in a typical three-electrode H-type cell setup. The linear sweep voltammetry (LSV) indicates a remarkable change in current densities in the presence of nitrates, confirming the reduction of nitrate. The intense absorption peak in UV Vis analysis of electrolytes analysis after Indophenol Blue (IB) processing confirmed the formation of ammonia. In the next phase, we plan to include potential metals and make their composites with different functionalized MXenes. Metals are excellent for nitrate reduction due to their high electrical conductivity and optimal binding energy with nitrate intermediates, enabling efficient and selective multi-electron transfer reactions. When combined with MXene, it provides enhanced active sites, conductivity, and stability for electrocatalytic performance.

# Recovery, Restoration and Interface Modification of Glass Fiber From Waste Composite Materials

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Abstract: The sustainable recovery and reuse of glass fibers from waste composite materials offer a promising solution to reducing environmental impact while conserving valuable resources. This study explores advanced interfacial modification to enhance the bonding efficiency in glass fiber-reinforced polyester composites. Aqueous suspension deposition was employed to coat recovered glass fibers from waste composite materials with commercially carboxylic acid-functionalized single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) to enhance fiber-matrix interfacial adhesion in polyester composites. A comprehensive analysis using single fiber fragmentation testing (SFFT), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, contact angle measurement, and Weibull statistical modeling demonstrated a significant enhancement in interfacial shear strength (IFSS) through CNT-based surface modification. Pristine glass fibers exhibited an IFSS of 30 MPa. In contrast, fibers treated with 0.0069 wt% SWCNTs achieved a remarkable IFSS of 62.5 MPa, while those coated with 0.0046 wt% MWCNTs showed an increase to 38.3 MPa. Notably, pyrolyzed fibers, which underwent thermal treatment, demonstrated the highest IFSS of 80.2 MPa. These findings highlight the transformative potential of CNT-modified glass fibers in creating highperformance, sustainable composite materials, paving the way for next-generation structural applications.

# Hydrothermal Synthesis and Photocatalytic Performance of Pure and Ce-Doped CdS Quantum Dots for Solar-Driven Applications

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## Presenting Author: Hafsa Bibi

Abstract: Cadmium sulfide (CdS) quantum dots (ODs) are widely studied for photocatalytic applications due to their excellent optical properties and ability to harness solar energy. However, challenges such as rapid charge recombination limit their efficiency. Rare-earth doping, particularly with cerium (Ce), has emerged as a promising strategy to enhance charge separation and improve photocatalytic performance. Objectives: This study aims to synthesize and investigate the structural, optical, and photocatalytic properties of undoped and Ce-doped CdS QDs to evaluate the effect of Ce doping on their efficiency in solar-driven photocatalysis. Methods: CdS QDs were synthesized using a hydrothermal method, with cerium incorporated as a dopant. Structural characterization was performed using X-ray diffraction (XRD) to confirm phase purity. Raman spectroscopy was employed to analyze vibrational modes and assess crystallinity. Optical properties were studied via UV-Vis spectroscopy and photoluminescence (PL) to determine bandgap modifications and charge carrier dynamics. The photocatalytic performance was assessed by monitoring the degradation of organic pollutants under simulated solar irradiation. Results: Ce-doped CdS QDs exhibited red shifts in absorption, reduced bandgap energy, and enhanced charge carrier separation compared to undoped CdS. Photocatalytic experiments demonstrated significantly improved degradation rates for Cedoped CdS, attributed to reduced electron-hole recombination and improved charge transport. These findings highlight the potential of Ce-doped CdS QDs for sustainable photocatalytic applications.
# Comparison of Organic/Inorganic Dielectric on the Performance pf DPPDTT Based Organic Field Effect Transistors

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Presenting Author: Waisfa Zulfiqar

**Abstract:** Low operational stability and undesirable shifts in electrical properties under ambient conditions remains significant challenges in commercialization of organic field effect transistors.in this study,we report an improvement in the operational stability of solution-processable polymer DPPDTT based OFETs by employing different gate dielectric configurations. Two types of devices were fabricated using bare Si<sub>3</sub>N<sub>4</sub> as gate dielectric which exhibits a higher density of interfacial traps and incorporating an additional layer of PVA along with Si<sub>3</sub>N<sub>4</sub> which reduces interfacial trap density. The OFET with PVA layer demonstrates superior performance, with a threshold voltage around 11V, mobility ~2.4\*10^{-3} cm2/V.s and a current on/off ratio in the range of 0.48 \* 10^4.performance measurements indicate that device with lower trap density exhibits improved electrical stability, while the device with higher trap density shows greater degradation over time. The reported findings provide a viable approach to enhancing the long-term stability of OFETs in ambient conditions through the strategic use of gate dielectric.

# Enhancing the Electrochemical Properties Of Co-MOF Using Mixed Ligands For Energy Storage and Watersplitting Applications

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Abstract: With the growing global demand for clean and sustainable energy, research on advanced materials for energy storage and conversion particularly, supercapacitors and electrochemical water splitting, has gained significant attention. However, the supercapacitor's low energy density and the slow reaction kinetics of electrochemical water splitting remain challenges. Transition metal-based electrodes are studied for their variable oxidation states and catalytic activity, but metal-organic frameworks (MOFs) offer advantages such as high porosity, stability, and enhanced catalytic activity. This study introduces a sonochemical synthesis approach for a novel mixed-ligand Co-MOF using pyromellitic acid (PMA) as the primary ligand and terephthalic acid (TPA) as the co-ligand. Three Co-MOFs – Co-MOF-PMA (S1), Co- MOF-TPA (S2), and CO-MOF-PMA, TPA (S3) - were synthesized and evaluated. XRD confirmed the successful synthesis of S3, while SEM revealed a porous, flake-like structure with multiple active sites. S3 exhibited outstanding energy storage performance, achieving a specific capacity of 520 Cg<sup>-1</sup> and a capacitance of 762 Fg<sup>-1</sup> at 1.0 Ag<sup>-1</sup>, respectively. An asymmetric S3//AC device delivered 64 Whkg-1 energy density at 1.3 Ag<sup>-1</sup> and 7659 Wkg<sup>-1</sup> power density at 9.0 Ag<sup>-1</sup>. For electrocatalysis, S3 demonstrated low HER and OER overpotentials of 150 mV and 50 mV at 10 mAcm-2, respectively, with significantly enhanced electrochemically active surface area (ECSA) of 190 cm2 (HER) and 651 cm2 (OER). This work presents a novel mixed ligand Co-MOF with promising potential for energy storage and watersplitting applications.

# N-doped Mesoporous Carbon Supported Dual-Metal Atom M-N-C Desert Rose Structure as an Effective Bifunctional Electrocatalyst For Zinc-Air Battery

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### Presenting Author: Uswa Arooj

**Abstract:** Slow oxygen reduction and oxygen evolution process are the two issues that prevent zinc air batteries from being used commercially. Nobel metal based electrocatalysts are being used commercially but their scarcity, high-cost and instability reduces efficiency of rechargeable zinc-air batteries. Single-atom site catalysts are commonly employed in electrocatalysis due to their high atomic efficiency. However, their single-metal structure limits multi-electron processes. Dual-atom sites (DASs) provide a viable alternative since neighboring active sites can improve catalytic efficiency through synergistic effects. This study introduces a nitrogen-doped mesoporous carbon (NMC) material decorated with dual-metal atoms. The Co-Mn/N-MC, was prepared using a template -assisted casting, demonstrated a notable ORR half-wave potential (E1/2) of 0.85 V, superior OER activity with an over potential of 360 mV at 10 mA/cm<sup>2</sup> with Tafel slope of 55 mV/dec. This improved performance results from the synergy among cobalt and manganese atoms within the NMC structure, suggesting that Co-Mn/N-MC is a highly effective candidate for advancing rechargeable ZAB technology. This work gives a strategy to synthesize and develop dual atom based multiple active sites for advanced electrolysis

# Fe Mn and Co Based Efficient Bifunctional Electrocatalyst Derived From MOF/ZIF For Oxygen Electrode in Zinc-Air Batteries

### Jaria Zahra

### USPCASE. NUST

Abstract: Zinc-air batteries (ZABs) have gained significant attention in renewable energy due to their exceptional safety, affordability, higher theoretical energy density (1084 Wh·kg<sup>-1</sup>), and environmental sustainability. The sluggish rate of oxygen electrolysis requires noble metalbased catalysts for rechargeable zinc-air batteries (RZABs), but these are expensive and exhibit instability issues. This requires the design of economical, highly stable, and efficient non-noble metal dual-functional electrocatalysts for oxygen reduction (ORR) and oxygen evolution (OER) reactions. We introduce an easy method to synthesize a trimetallic nitrogen-doped nanoporous carbon (FeMnCo/N-C) electrocatalyst. By combining Fe/Mn-MOF with ZIF-67, followed by pyrolysis, we receive FeMnCo/N-C. This electrocatalyst, featuring a high surface area, reveals exceptional bifunctional activity, with half-wave potential (E1/2 = 0.83V) for the oxygen reduction reaction (ORR) and potential at 10mA/cm2(Ej (10) = 1.60V) for the oxygen evolution reaction (OER), which results in a potential gap of 0.77V, exceeding Co/N-C and Fe/Mn-C. It has improved stability compared to Pt/C and RuO2. The bifunctional activity of an electrocatalyst is due to the combined effects of the tri-metals, nitrogen-doped carbon, and its porous nature, offering FeMnCo/N-C a notable candidate for enhancing effectiveness and longterm sustainability of rechargeable zinc-air battery technology.

#### Dual vapor deposited W2N/WC/CNTs

Tooba kalsoom, Ghulam ali, Nisar Ahmed

### USPCASE, NUST

#### Presenting Author: Tooba kalsoom

Abstract: This study explores the electrochemical performance of tungsten nitride (W2N) thin films and carbonized tungsten nitride thin films as electrode in supercapacitors. W2N thin films are synthesized by physical vapor deposition method (PVD). After that, prepared W2N thin films are carbonized via chemical vapor deposition method (CVD). A significant increase in capacitance is observed after carbonization due to an increase in surface area and electrical conductivity with the capacitance rising from 23.54F/cm<sup>2</sup> for W2N to 66.26F/cm<sup>2</sup> for W2N-CNTs. Morphological, structural and electrochemical analysis of prepared thin films is conducted using scanning electron microscopy (SEM), x-ray diffraction (XRD) and cyclic voltammetry (CV) respectively. The results show that carbonization has significantly improved the electrochemical performance of W2N thin films resulting in enhanced stability during charge discharge cycles, increased capacitance and greater energy storage efficiency. Moreover. SEM images confirm the presence of carbon nanotubes (CNTs) on thin film surface which increases the overall surface area. This study highlights the potential of tungsten nitride thin films as electrode material in high performance supercapacitors. Overall, W2N-CNTs outperform W<sub>2</sub>N, making them a promising candidate for next-generation energy storage devices. This study aims to evaluate and compare the electrochemical performance of W<sub>2</sub>N and W2N-CNT composites as supercapacitor electrodes, focusing on how the addition of CNTs influences capacitance, charge transfer, and overall efficiency. Keywords: Tungsten nitride, thin films, Chemical vapor deposition, Physical vapor deposition, Carbonization

## Coupling Ceramic Membrane Filtration and Granular Activated Carbon Adsorption for Effective Treatment of Paper Mill Effluent

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### Presenting Author: Aisha Syed

Abstract: The effluent of the targeted paper industry contains pollutants and becoming a significant environmental concern and violating the Environmental Protection Agency (EPA) guidelines. To meet the EPA standards and overcome environmental challenges, a submerged ceramic membrane reactor integrated with the adsorption effect of granular activated carbon (GAC), was operated for treating paper industrial wastewater. The effect of GAC having different shapes (cylindrical & irregular) for their scouring effect on membrane surface was also studied to enhance removal efficiency and mitigate the fouling rate of the membrane. The effluent from the Horizon Paper Industry was first subjected to sedimentation as a pretreatment to reduce turbidity and to maximize the paper recovery. This pretreatment also facilitates turbidity and COD profiles assessment. Then the supernatant of this pretreated wastewater was collected and analyzed for further treatment in the submerged fluidized ceramic membrane reactor (SCMR). The GAC particles were fluidized along the membrane surface through bulk recirculation. An alumina-coated ceramic membrane was used to treat paper industry wastewater under different flux modes of filtration. The flow rate was set at 11 L m<sup>-2</sup> h<sup>-1</sup> with and without GAC particles. The fouling rate was recorded as 0.223 bar and 0.73 bar with and without GAC, regardless of the effect of flux. The organic removal rate was significantly enhanced by the fluidization of activated carbon, reaching 99%. This study accentuates the prospect of integrating ceramic membranes with GAC for sustainable industrial wastewater treatment. Moreover, it also evaluates the effect of different GAC grades on flux stability and membrane longevity, providing perceptions for optimizing operational conditions.

### Circular Economy "Restoration and Recovery of Glass Fibers "

# Syeda Mehak Ali Kazmi, Zohaib Ifftikar, Qazi Mujtaba Saleem, Sana Ghaffar, Muhammad Irfan

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### Presenting Author: Syeda Mehak Ali Kazmi

Abstract: Glass fiber have attracted extreme attention due to the distinct exclusive privileges such as their use in various industries, construction, automotive and aerospace. However, management of glass fiber composite waste is a critical issue for environment and the ecosystem, so recycling of glass fibers is the major consideration for researchers. Among various recycling methods, mechanical and thermal treatments(e.g. pyrolysis and post Oxidation) and other chemical methods have been studied, but it often leads to a loss of mechanical properties and fiber strength. To overcome these limitations, this study proposes a coating-based approach to enhance the interfacial strength of glass fibers, thereby improving their mechanical properties and durability. For this, the surfaces of glass fiber is being modified using polyurethane coating, changing different parameters like concentration, time, and solvent. When polyurethane (acting as a foaming agent) is applied, bead-like structures form on the fiber surface, enhancing interfacial strength, improving adhesion and overall performance. Different characterization test are being carried out such as scanning electron microscope (SEM), Fourier Transform Infrared Spectroscopy, Raman Spectroscopy optical microscopy, and Tensile test. The average tensile strength of the glass fibers was around 1 GPa. The distribution in strength of glass fibers is referred to by using Weibull distribution. This study offers a viable, eco-friendly glass fiber recycling solution by enhancing its mechanical strength and durability using a straightforward yet efficient coating method.

## Freeze-Dried Microneedle Patches for Transdermal Insulin Delivery

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### Presenting Author: Ali Khan

Abstract: Microneedle-based transdermal drug delivery systems have gained significant attention due to their minimally invasive nature and potential for enhancing drug bioavailability. In our ongoing project, we present freeze-dried microneedle patches designed for the controlled transdermal delivery of insulin, aimed at improving patient compliance and therapeutic efficacy. The microneedles will be composed of a biocompatible polymer matrix (Hyaluronic Acid/Sodium Alginate) crosslinked with calcium chloride to enhance mechanical strength and stability. The freeze-drying process is expected to ensure rapid dissolution upon skin penetration, enabling efficient drug release. Fabrication follows a micro-molding approach, starting with 3D-printed master molds to achieve precise needle geometries. The microneedle arrays will be evaluated for structural integrity using scanning electron microscopy (SEM) and mechanical strength through compression testing. In vitro penetration studies will be conducted using artificial skin models, followed by drug release analysis to assess diffusion kinetics. The expected outcomes include mechanically robust microneedles capable of effective skin penetration, sustained insulin release, and improved bioavailability compared to conventional delivery methods. This ongoing research aims to optimize key formulation parameters to enhance drug loading efficiency, dissolution behavior, and patient usability. Future work will focus on refining polymer composition, conducting in vivo validation, and exploring clinical feasibility. By integrating material science and biomedical engineering, this study contributes to advancing transdermal drug delivery technologies for improved diabetes management.

### **PP21**

# Synthesis of Multi-Metal Doped CaO Catalyst from Chicken Eggshells for Biodiesel Production

Faseeha Ashraf

#### UMT Lahore

### Presenting Author: Faseeha Ashraf

Abstract: Energy is the primary and the most essential need for life. Major source of energy around the globe is fossil fuel. As world energy requirement is raising every day, amount of fossil fuels is decreasing. In order to achieve the current energy demand, world is shifting toward the renewable resources of energy. This study is concerned with the synthesis of biodiesel using waste cooking oil with calcium oxide catalyst (CaO) from waste eggshells. All experiments were performed in laboratory. Eggshells were washed, dried and crushed thoroughly and then calcined at 900°C. To enhance the catalytic activity, catalyst was doped with Cu(NO3)<sub>2</sub> and Co(NO3)<sub>2</sub> by using co- precipitation method. Meanwhile, waste cooking oil was filtered to remove impurities. Transesterification reaction was used for biodiesel synthesis. Alcohol to oil ratio was same in all reaction cycles i.e. 1:20 while different weight percentages of catalyst concentration were taken (5wt%, 10wt%, 15wt%, 20wt% and 25wt%). Reusability of catalyst was also checked with two catalyst concentrations (20wt% and 25wt%). Reaction duration was 4 h with 65°C temperature. Characterization analysis was performed by XRD, SEM, FTIR techniques for catalyst analysis and GC/MS for biodiesel sample. This study opened a new avenue for researchers to make biodiesel with the use of waste material. Fuel crisis across the world can be overcome if this research would Considered at commercial scale.

# Tuning Photo-Catalytic Activity Of ZnO Via Transition Metal Doping (Ni,Co) Under Visible Light Spectrum

Usman Amir, Zainab Zahra, Muhammad Umar Saleem

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Presenting Author: Usman Amir

Abstract: This project investigates the optimization of ZnO for photocatalysis under visible light through doping of nickel and cobalt. The purpose of this study is the treatment of waste water by experimenting with organic dye i.e. methylene blue. The efficacy of pure zinc oxide as a photo catalyst experiences a disappointing drop under visible light due to its wide band gap. Doping provides a modification route to alter this electronic property of ZnO. Nickel and Cobalt have similar ionic size to zinc lessening lattice distortion even at relatively high dopant concentration. Both transition metal elements are n dopants having a positive effect on the bandwidth of ZnO. Pure ZnO for control was compared with doped ZnO with varying dopant concentrations in a degradation study. ZnO was synthesized using co-precipitation method and results were verified via different characterization techniques i.e. XRD, SEM, FTIR, and UV-Vis. XRD data determined the successful synthesis of highly crystalline ZnO having crystallite size between 15-30 nm. The UV-Vis was primarily utilized to interpret the change in transmittance as the affected efficiency of degradation as a result of improved bandwidth of ZnO. The doping was expected to affect the crystallite size and bandwidth improving the charge carrier recombination and radical generation rate during solar driven degradation of methylene blue dye.

### **PP23**

### Defect Chemistry and Thickness Effect on Electrostrain in Lead Free KNN Ceramics

Muhammad Wasim, Antonio Feteira, Evangelos Kordatos and Iasmi Sterianou

#### Sheffield Hallam University

#### Presenting Author: Muhammad Wasim

**Abstract:** K0.5Na0.5NbO3-based ceramics are among the most studied Pb-free piezoceramics, as potential contenders to replace piezoelectric actuators based on hazardous Pb(Zr,Ti)O3 ceramics. For these applications, the magnitude and the temperature stability of the electric field induced strain is of para-mount importance. A significantly large number of research efforts ranging from chemical doping of K0.5Na0.5NbO3 ceramics to microstructural texturing have been reported over the last two decades as different approaches to tailor their piezoelectric performance. Recently it was reported that Sr-doped K0.5Na0.5NbO3 ceramics can exhibit a so-called giant electric field induced strain exceeding 1%. This surprising-ly large response is revisited in this work, using specimens prepared follow-ing the experimental procedures reported. In addition, to gather further in-sights from a doping concept based on Asite replacement, other divalent species, such as Ca and Ba were employed in the fabrication of K0.5Na0.5NbO3-based ceramics. In this study, we compare the electric field induced polarisation and strain of those ceramics and establish their basic crystal chemistry.

# Design and Development of Ion Exchange Method For Strength Restoration of Recycled Glass Fibers

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### Presenting Author: Iman Fatima

Abstract: The extensive use of glass fibers in composites across industries such as aerospace, automotive, construction, and sports has highlighted their superior mechanical properties, including high tensile strength, lightweight characteristics, and resistance to environmental degradation. However, the sustainability of these materials is compromised by the lack of effective recycling methods, leading to significant waste generation. Discarded glass fibers exhibit deteriorated mechanical properties, limiting their reuse and contributing to environmental concerns. Addressing this challenge is vital to advancing sustainable materials engineering practices. Our Final Year Project (FYP) seeks to restore the mechanical strength of recycled glass fibers, specifically E-glass fibers, through an innovative ion exchange process. The restoration process involves replacing sodium ions on the surface of degraded glass fibers with potassium ions, thereby enhancing their strength and reusability. This approach presents a sustainable and cost-effective solution to mitigate the waste generated by glass fiber composites. The methodology involves the preparation of supersaturated potassium nitrate solutions, followed by immersing the recycled glass fibers in these solutions at controlled temperatures. Key parameters such as immersion time, temperature, and solution concentration were optimized through systematic experimentation. The ion exchange process was validated using advanced analytical techniques, including scanning electron microscopy (SEM) for surface morphology, energy-dispersive X-ray spectroscopy (EDS) for compositional analysis, and mechanical testing to evaluate tensile strength restoration. Experimental results demonstrated significant improvements in mechanical properties. The highest average strength of 2399.13 MPa was achieved for fibers treated under 30 minutes of salt treatment (ST) with normalization, indicating a substantial enhancement compared to pristine fibers (1123.64 MPa). Additionally, the annealing condition of 30 minutes following 30 minutes of ST yielded an average strength of 1263.30 MPa, further supporting the effectiveness of the ion exchange process in restoring fiber strength. These findings highlight the potential of this method in extending the life cycle of glass fibers and promoting sustainable composite manufacturing.

# Designing and Development of High-Performance Self-Healing Nanocomposite Sizings for Enhancing Mechanical Properties of Recycled Glass Fibers

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### Presenting Author: Eisha Hammad

Abstract: This project focuses on efficiently recycling glass fibers from end-of-life (EoL) glass fiber-reinforced polymers (GFRPs) to develop high-performance self-healing materials. GFRPs are widely used in aerospace, automotive, construction, and renewable energy industries due to their excellent strength-to-weight ratio, durability, and corrosion resistance. However, their non-biodegradable nature poses significant environmental challenges, with over two million metric tons of GFRP waste generated annually in the U.S., much of which is landfilled or incinerated. Traditional recycling methods suffer from high energy consumption and mechanical property degradation, necessitating innovative approaches to retain or enhance fiber quality for reuse. This study explores thermal recycling (pyrolysis), chemical treatments, and surface modification with carbon nanotubes (CNTs) to improve recycled fiber properties. Additionally, microcapsule synthesis is employed to enhance self-healing capabilities. Advanced characterization techniques, including SEM, tensile strength testing (ASTM-D1557), and Weibull analysis, assess fiber performance. A total of 20 samples per condition were analyzed for consistency. Results show that CNT-coated recycled fibers exhibit superior mechanical properties, with tensile strength reaching 1684.87 MPa at 0.0069 g of single-walled CNTs-improving by 149.9% and 133.4% over pristine and pyrolyzed fibers, respectively, with a standard deviation of 1.09 GPa. These findings highlight a sustainable recycling approach that enhances fiber quality, enabling their reuse in high-performance applications and reducing the environmental impact of GFRPs.

# Advanced Cellulose Triacetate-Based Mixed Matrix Membranes Enhanced by Cu-BTC MOFs for Carbon Capture

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#### Presenting Author: Esha Asad

Abstract: Cu-BTC (HKUST-1) metal-organic framework (MOF) is widely acknowledged for its ability to capture CO<sub>2</sub>, attributable to its unsaturated copper sites. Additionally, its crystalline structure and selective pores attract polar CO<sub>2</sub> molecules, providing excellent CO<sub>2</sub> separation performance. This study focused on developing mixed matrix membranes (MMMs) based on cellulose triacetate (CTA), incorporating Cu-BTC and bimetallic Ni-Cu-BTC MOFs for CO<sub>2</sub>/CH<sub>4</sub> separation. CTA was chosen as the polymer matrix due to its economical and green nature. The optimized membrane, containing 10 wt.% Ni-Cu-BTC, showed a CO<sub>2</sub> permeability of 22.95 Barrer at 25 °C and a transmembrane pressure of 5 bar. These results represent more than a two-fold increase compared to the pristine polymer, with a superior CO<sub>2</sub>/CH<sub>4</sub> selectivity of 33.75. The improvement in gas separation performance is attributed to a 51.66% increase in fractional free volume (FFV), a 49.30% rise in the solubility coefficient, and a 51.94% boost in the diffusivity coefficient compared to the pristine CTA membrane. Furthermore, the dualsorption model analysis revealed that the enhanced CO<sub>2</sub> solubility in the optimized membrane is driven by a 14.81% improvement in Henry's coefficient (KD), a 15.04% increase in the Langmuir capacity constant (C'H), and a 65% rise in the hole affinity constant (b). Therefore, the fabricated membranes highlight the effectiveness of CTA/Ni-Cu-BTC for CO<sub>2</sub> separation, making them promising materials for natural gas processing and related applications.

# Comparative Assessment and Optimization of Natural and Synthetic Coagulants For Real Food Industrial Wastewater Treatment

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### Presenting Author: Tuba Safdar

Abstract: The discharge of untreated industrial wastewater into freshwater bodies is causing a significant environmental threat, endangering aquatic life and deteriorating water quality. This study compares both natural and synthetic coagulants for food industries wastewater at Hattar Industrial Estate. Traditionally, inorganic coagulants such as alum, ferric chloride, and polyelectrolytes are employed in coagulation-flocculation processes. In this study, Polyaluminium chloride (PACl) and Guar gum, representing synthetic and natural coagulants, respectively were evaluated. Guar gum, a biopolymer derived from the seeds of Cyamopsis tetragonoloba, is an economical and environmentally benign alternative that has demonstrated efficacy in the removal of heavy metals, bentonite suspensions, and landfill leachate. Experimental findings revealed that when used as a coagulant aid alongside alum, Guar gum achieved 83% turbidity removal, 49% total suspended solids (TSS) reduction, and a 33% decrease in chemical oxygen demand (COD) at optimal dosage. However, PACl exhibited superior performance, achieving 1.5 times greater COD removal, particularly at lower concentration. Regardless of the enhanced removal efficiency of synthetic coagulants, the use of natural coagulants presents distinct advantages. Given concerns regarding residual aluminum concentrations in case of PACl, natural coagulants such as Guar gum present a sustainable and environmentally friendly alternative for wastewater treatment in the food industry.

# Flow Analysis of Double Circular Cylinders Placed Side by Side through Particle Image Velocimeter (PIV) using Nano Glass Particles

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Abstract: In current study, time averaged and instantaneous flow structure for two circular cylinders placed side by side was investigated using particle image Velocimeter (PIV). Nano particles of glass were used as seeding particles to trace the movement of the fluid owing to their small size, hollow structure, greater scattering efficiency, and their ability to illuminate when a beam of light is incident upon them. The diameter of 12.5 mm was same for both the cylinders. The flow under consideration had a Reynolds Number of 3600. The flow was rendered laminar for ease and it was done by using built in honey comb structure in PIV. Post processing involved following the contour of the Nano particles in the fluid using a high resolution camera. After the required post processing, the time averaged velocity data was plotted using Tec plot software and its contour was investigated. Moreover, this result was compared with the actual results of flow over an oval and it was assumed that these side by side cylinders behaved as a single oval. It was observed that the results of experimental and actual data were quite similar in nature.

# Techno-Economic Assessment of an Eco-Friendly Exhaust Capture Process for Fossil Fuel Power Plants

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Presenting Author: Gohar Ayub

**Abstract:** The rise in greenhouse gas emissions from fossil fuel-fired power plants is leading to the development of new technologies that improve CO<sub>2</sub> capture and sequestration (CCS). Oxy fuel combustion is a better option among different technologies because of a rapid rate of combustion, reduction in flue gas volume, low fuel consumption and near to zero CO<sub>2</sub> emissions. Oxygen purity for all cases will be 98 mol%. The models developed will be validated and verified with the already published literature. Moreover, the modelling of these power plants is realized in Aspen Plus at the gross power output of 768 MWe for oxy coal power plant and integrated with air separating unit and CO<sub>2</sub> compression and purification unit. Oxygen purity will be fixed at 98 mol%. The process performance, in terms of efficiency, emissions and potential losses for all the cases, is analyzed. Biomass exhibits higher fuel flow rates of 612 tonne per hour but lower net and boiler efficiencies compared to coal and natural gas. However, biomass offers lower fuel costs of \$13.89 per tonne and levelized costs of electricity (LCOE) of \$6 per MWh. The choice of energy source should balance cost considerations with resource availability and environmental impact. Coal and natural gas are economically favorable, whereas biomass delivers environmental benefits.

# Dual Metal-Based Nanomaterial Catalyst for Solvent-Free Cycloaddition of CO<sub>2</sub> to Epoxide

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### Presenting Author: Ali Hamza

Abstract: Fixation of CO<sub>2</sub> through cycloaddition reaction is the important and traditional method to convert them into cyclic carbonates which are used as a green solvent. Porous metalorganic frameworks (MOFs) are unique among the many catalytic systems because of their modular design, which increases stability and reusability following the many catalytic run. In this manner, the MOFs integrate unique capabilities that demonstrate significant carbon dioxide fixation efficiency. In order to determine the ideal composition to optimizing conversion efficiency in cycloaddition events, a green solvothermal approach is used to construct a series of bimetallic Zn/Zr metal-organic frameworks (MOFs). The characterization Zn/Zr MOFs is done to evaluate their morphologies and structures surface chemistry and thermal stability of Synthesized and regenerated sample by FTIR, XRD, SEM, TGA, XPS. Zno.75/Zro.25-MOF, demonstrates excellent catalytic activity for CO<sub>2</sub> cycloaddition with epoxides under mild conditions (2bar, 50°C, 4 hours) using TBAB as a co-catalyst in a solvent-free environment, achieving yields over 75%. Optimizing the reaction conditions (20 bar, 120°C, 6 hours) resulted in a highly impressive yield of 99% for the conversion of propylene oxide to propylene carbonate, showcasing the catalyst's strong efficiency. In the same manner, high productivities (>90%) were achieved for styrene oxide (SO) and epichlorohydrin (ECH). The MOF showed remarkable stability and reusability, even after five cycles, again the crystallinity, structure surface chemixstry of the material of the regenerated MOF is determined by XRD, FTIR, and XPS. This work highlights the potential of MOFs as efficient catalysts for CO<sub>2</sub> conversion, contributing to sustainable chemical processes.

# Development of High Temperature Oxidation Resistant Thermal Barrier Coating for Nickel Chromium Superalloys

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## Presenting Author: Muhammad Shafqat

Abstract: Thermal Barrier Coating (TBC) insulates stainless steels, which are commonly used for high-temperature applications. These TBCs' primary purpose is to shield the IC engine components (cylinder liner, piston) from temperatures above 1000C. TBCs, however, can fail for several reasons, including residual stresses, phase changes, sintering, hot corrosion attack, and oxidation deterioration, all of which have an adverse effect on their operational, thermal and mechanical capabilities. To further improve the toughness and durability of TBCs, a unique thermal barrier material and method must be developed. It is crucial to create coating solutions that can provide long-lasting oxidation protection and thermal barrier function for high Cr and Ni steels and alloys. Furthermore, coating techniques should be useful for producing protective layers on the interior and outer surfaces of large-scale components with intricate shapes. This study deals with the development of a novel thermal barrier coating that can perform well at above 1000 °C, Characterization of developed TBC for its microstructural and thermal properties. In comparison to traditional ceramic TBCs materials, the new coating is expected to form intermetallic after diffusing to the substrate surface, thereby changing the chemical composition of the surface and extending the lifespan of the substrate material at significantly higher temperatures (1200 °C). The innovative thermal barrier coatings with longer lifespans and higher operating temperatures will be required for application in the future on heavily loaded components like diesel engine combustion chambers and gas turbine blades and vanes. Microscopy, scanning electron microscopy (SEM) provided with energy dispersive X-ray spectrometry (EDS), and X-ray diffraction (XRD) and X-Ray Fluorescence (XRF) will all be used in this study to determine microstructural and chemical properties of the samples.

# Synthesis and Characterization of Bio-ceramic Loaded 3D Printed Scaffolds for Hard Tissue Engineering

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### Presenting Author: Usama Bin Razzaq

Abstract: Bone represents the dense and most mineralized form of connective tissue, serving as structural framework that supports and protects vital organs, ensuring their proper physiological function. Fractures or neoplasms result from trauma or pathology. Minor injuries heal via remodeling, while severe cases need surgical repair. Advancement in biomedical field led to various techniques in regenerating bone. In this study, advanced 3D printing technology was used to fabricate biocomposite scaffolds composed PLA loaded with calcium magnesium silicate (CMS) and silk fibroin microspheres (SFM). Prepared materials were extruded using a WELLZOOM filament extruder followed by 3D printing of scaffolds. The scaffolds were characterized using various progressive techniques. FTIR analysis confirmed the polymeric functional groups (C=O, C-O, O-Mg-O, O-Si-O, -NH) in scaffold. XRD analysis confirmed the crystallinity of the CMS prepared and composite synthesized. SEM analysis showed that increase in CMS percentage (10%-20%) resulted in increased porosity, roughness in surface and equal distribution of bioceramics and silk fibroin microspheres in scaffolds. Additionally, E. coli was shown to have antibacterial activity, demonstrating that the scaffolds inhibit bacterial development. According to in vitro degradation experiments, the composite scaffold showed a favourable degradation that matched the bone healing time, 28 days approximately. All studies converge on the conclusion that 3D-printed scaffolds play a pivotal role in facilitating bone regeneration.

## Selective Hydrogenolysis of Glycerol Using Co/Al<sub>2</sub>O<sub>3</sub>-based Catalysts

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Presenting Author: Muhammad Sajjad Haider

Abstract: Raw glycerol produced in massive quantities by the biodiesel and soap industries poses significant economic and environmental challenges. The catalytic hydrogenolysis of this glycerol to produce lower polyols, including 1,2-propanediol (1,2-PDO) and ethylene glycol (EG), is a strategically significant route for sustainable production of these valuable industrial chemicals. This process not only addresses the waste management problem caused by the abundance of raw glycerol but also reduces the reliance on conventional fossil fuels that are currently used to produce these polyols. In this work, Co/Al 2 O 3 -based catalysts were developed for the selective hydrogenolysis of glycerol to 1,2-PDO and EG. The catalysts were prepared using the wet impregnation technique, followed by drying, calcination, and reduction before the reaction. The synthesized catalysts were characterized using XRD, BET, SEM, and ICP techniques. The liquid-phase reaction was conducted in batch mode under elevated pressure and temperature conditions. Both the liquid- and gas-phase products were analyzed using gas chromatography. The effects of catalyst synthesis conditions and reaction conditions on catalytic activity and product selectivity were explored. A maximum glycerol conversion of 46% was obtained with an average liquid-phase selectivity of 42% and 6% toward 1,2-PDO and EG, respectively. The glycerol conversion and liquid-phase selectivity to 1,2-PDO were successfully correlated to catalyst structural characteristics, providing deeper insight into reaction chemistry and allowing rational catalyst design and predictable catalyst performance.

# Sustainable Production of Calcium Carbonate from Marble Waste Byproducts for Fertilizer and Chemical Industry

Muhammad Usman\*, Rana Muhammad Asad Khan, Ghufran Ur Rehman

Pak-Austria Fachhochschule Institute of Applied Sciences and Technology

## Presenting Author: Muhammad Usman

Abstract: Pakistan possesses an extensive and substantial reserve of marble amounting to an impressive 300 billion tons; however, it is noteworthy that approximately 60% of this valuable resource is rendered as waste during the intricate processes of marble cutting and polishing activities, which raises significant concerns regarding resource efficiency and environmental sustainability. The composition of marbles is mainly composed of calcium carbonates (42 to 45 %) and magnesium carbonates (2 to 3%) with some impurities. To reduce the harmful environmental effect associated with marble waste generated from mining and processing operations, an experimental study has been conducted that has meticulously investigated the multifaceted process of synthesizing precipitated calcium carbonate (PCC) for industrial applications from marble waste, employing a systematic approach that encompasses calcination, hydration, and carbonation techniques. The calcination efficiency was examined at the temperature of 1050 °C for particles sizes of -26.5+9.5 mm and -9.5+0.355 mm and slaking experiments are carried out lime to distilled water ratio (1:3.5) for all different particle sizes. The broad objective of this investigation has to substantially diminish the adverse effects that arise from marble waste extraction and processing, while simultaneously enhancing the practices of waste management within quarry operations, ultimately culminating in the production of high-purity PCC that can be utilized in the formulation of fertilizers.

# Development of Nanomaterials Based Electrochemical Arsenic Detection System For Drinking Water

Ali Hassan Paracha, Anosh Ehsan, Muhammad Imran

Department of Mechanical Industrial and Energy System (DMIES) University of Sargodha

### Presenting Author: Ali Hassan Paracha

Abstract: Numerous health conditions, including skin cancer, lung and bladder cancer, cardiovascular disease, hyperkeratosis, dermal lesions, and various skin disorders, can be brought on by prolonged exposure to arsenic in drinking water. The World Health Organization (WHO) has determined that 0.01 mg/L of arsenic is the acceptable limit for drinking water. The goal of our study is to make a portable electrochemical device that can detect arsenic in drinking water till sub ppm levels. Carbon nanotubes (CNTs) and its composites with Iron Oxide Nanoparticles is used as a sensing material in developed electrochemical arsenic sensor. The working and counter electrode of the three-electrode configurations are composed of carbon, while the reference electrode is made of Ag/AgCl. An open source potentiostat is fabricated and used for electrochemical characterization of developed sensing system. Cyclic voltammetry and chronoamperometric test is used to detect various levels of arsenic in drinking water. The developed electrochemical sensor demonstrated a detection limit of 7 ppb, with a sensitivity of 0.9  $\mu$ A/ppb. The device showed a rapid response time of 15 seconds, ensuring efficient arsenic detection. The results confirm the potential of the sensor for real-time arsenic monitoring in drinking water.

# Development Of Portable and Wireless Potentiostat For Arsenic Detection In Drinking Water

## Anosh Ehsan, Ali Hassan Paracha, Muhammad Imran

## Department of mechanical industrial and energy system, University of Sargodha

### Presenting Author: Anosh Ehsan

Abstract: Numerous health conditions, including skin cancer, lung and bladder cancer, cardiovascular disease, hyperkeratosis, dermal lesions, and various skin disorders, can be brought on by prolonged exposure to arsenic in drinking water. The World Health Organization (WHO) has determined that 0.01 mg/L of arsenic is the acceptable limit for drinking water. The goal of our study is to make a portable wireless potentiostat that can detect arsenic in drinking water till sub ppm levels.. An open source potentiostat is fabricated and used for electrochemical characterization of developed sensing system. Cyclic voltammetry and chronoamperometric test is used to detect various levels of arsenic in drinking water. The developed potentiostat is able to detect signals upto sub ppm level of arsenic with high signal to noise ratio. A potentiostat-based system offers the advantage of high sensitivity and selectivity when paired with electrochemical sensors. Making this system portable and wireless allows for easy field deployment and rapid detection without the need for laboratory settings. The developed system demonstrated a detection limit of 7 ppb, with a sensitivity of 0.9 µA/ppb. The device showed a rapid response time of 15 seconds, ensuring efficient arsenic detection. The results confirm the potential of the sensor for real-time arsenic monitoring in drinking water.

# Fluorescence Based Detection Of Industrially Important and Hazardous 4-Nitrophenol in Real Sampless: A combination of Extensive optical and theoretical studies

### Khanzadi Omama Khan

Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus

## Presenting Author: Khanzadi Omama Khan

Abstract: A triphenylamine (TPA) based fluorescent sensor T-TPA was elaborately designed which exhibited high quantum yield (QY). The sensor T-TPA displayed aggregation induced emission enhancement (AIEE) character that was confirmed by dynamic light scattering (DLS) analysis. The AIEE active  $\pi$ -electron rich sensor bearing thiourea moiety was employed for the detection of 4-nitrophenol (4-NP) in solution as well as vapor phase. In solution, sensor displayed fluorescence "turn-off" response towards 4-NP that was attributed to photoinduced electron transfer (PET). The quenching response of sensor T-TPA against 4-NP was highly selective even in the presence of higher concentration of interferences. The mechanistic approach for 4-NP sensing was confirmed through 1H NMR titration experiment, UV-Vis absorption spectroscopy, dynamic light scattering (DLS), and density functional theory (DFT) methodologies. Moreover, non-covalent interaction (NCI) and Bader's quantum theory of atoms in molecules (QTAIM) analysis was performed to support the presence of non-covalent interactions. Furthermore, the sensor was employed for the detection of 4-NP in industrial waste and lake water samples. Additionally, sensor coated paper strips were prepared to do the contact mode detection of 4-NP. Finally, the fluorescence quenching response of sensor was used for the fabrication of logic gate.

# Development of Nanomaterials Based Electrochemical Arsenic Detection System For Drinking Water

### Ali Hassan Paracha

Department of Mechanical Industrial and Energy System (DMIES), University of Sargodha

### Presenting Author: Ali Hassan Paracha

Abstract: Numerous health conditions, including skin cancer, lung and bladder cancer, cardiovascular disease, hyperkeratosis, dermal lesions, and various skin disorders, can be brought on by prolonged exposure to arsenic in drinking water. The World Health Organization (WHO) has determined that 0.01 mg/L of arsenic is the acceptable limit for drinking water. The goal of our study is to make a portable electrochemical system that can detect arsenic in drinking water upto sub ppm levels. Carbon nanotubes (CNTs) and its composites with Iron Oxide Nanoparticles is used as a sensing material in order to develop electrochemical arsenic sensor. The working and counter electrode of the three-electrode configurations are composed of carbon, while the reference electrode is made of Ag/AgCl. An open source potentiostat is fabricated and used for electrochemical characterization of developed sensing system. Cyclic voltammetry and chronoamperometric test issued to detect various levels of arsenic in drinking water. The developed electrochemical sensor demonstrated a detection limit of 7 ppb, with a sensitivity of 0.9  $\mu$ A/ppb. The device showed a rapid response time of 15 seconds, ensuring efficient arsenic detection. The results confirm the potential of the sensor for real-time arsenic monitoring in drinking water.

# Development of a Portable and Wireless Potentiostat For Arsenic Detection in Drinking Water

### Anosh Ehsan

# Department of Mechanical, Industrial and Energy system (DMIES), College of Engineering and Technology, University of Sargodha

### Presenting Author: Anosh Ehsan

Abstract: Prolonged exposure to arsenic in drinking water poses severe health risks, including skin, lung, and bladder cancer, cardiovascular diseases, and dermatological disorders. This study focuses on the fabrication of a portable wireless potentiostat for real-time arsenic detection in water samples. An open-source potentiostat was developed using a compact, low-power electronic design integrated with a wireless communication module for remote monitoring. The system was optimized for high signal stability, low noise, and efficient electrochemical measurements. The fabricated potentiostat was interfaced with an electrochemical sensor to perform cyclic voltammetry (CV) and chronoamperometry (CA) for arsenic detection. Experimental validation demonstrated that the potentiostat achieves a detection limit of 7 ppb with a sensitivity of 0.9  $\mu$ A/ppb. The device offers a rapid response time of 15 seconds, and reliable wireless data transmission, making it suitable for field applications. The integration of miniaturized hardware and wireless connectivity enables efficient arsenic monitoring without the need for laboratory-based equipment. The developed portable potentiostat presents a cost-effective and scalable solution for real-time arsenic detection, contributing to improved water quality monitoring and public health safety.

# Synthesis of Multi-Metal Doped CaO Catalyst from Chicken Eggshells for Biodiesel Production

Faseeha Umair

University of Management and Technology, Lahore

Presenting Author: Faseeha Umair

**Abstract:** Energy is the primary and the most essential need for life. Major source of energy around the globe is fossil fuel. As world energy requirement is raising every day, amount of fossil fuels is decreasing. In order to achieve the current energy demand, world is shifting toward the renewable resources of energy. This study is concerned with the synthesis of biodiesel using waste cooking oil with calcium oxide catalyst (CaO) from waste eggshells. All experiments were performed in laboratory. Eggshells were washed, dried and crushed thoroughly and then calcined at 900°C. To enhance the catalytic activity, catalyst was doped with Cu(NO<sub>3</sub>)<sub>2</sub> and Co(NO<sub>3</sub>)<sub>2</sub> by using co- precipitation method. Meanwhile, waste cooking oil was filtered to remove impurities. Transesterification reaction was used for biodiesel synthesis. Alcohol to oil ratio was same in all reaction cycles i.e. 1:20 while different weight percentages of catalyst concentration were taken (5wt%, 10wt%, 15wt%, 20wt% and 25wt%). Reusability of catalyst was also checked with two catalyst concentrations (20wt% and 25wt%). Reaction duration was 4 h with 65°C temperature. Characterization analysis was performed by XRD, SEM, FTIR techniques for catalyst analysis and GC/MS for biodiesel sample. This study opened a new avenue for researchers to make biodiesel with the use of waste material. Fuel crisis across the world can be overcome if this research would consider at commercial scale.

# Development of Cost-Effective Photocatalytic Ceramic Membranes for Enhanced Wastewater Treatment and Fouling Resistance

## Syed Taufiq Ahmad

Department of chemical and Energy Engineering PAF-IAST, Haripur, Khyber Pakhtunkhwa.

### Presenting Author: Syed Taufiq Ahmad

Abstract: The increasing demand for freshwater, propelled by growing industries and population growth, requires innovative approaches to wastewater treatment. Membrane technology presents certain advantages; however, it is constrained by fouling, which results in increased operational costs and diminished efficiency. This research tackles these challenges by creating economical photocatalytic ceramic membranes (CMs) utilizing mineral-based supports like pyrophyllite and incorporating titanium dioxide (TiO<sub>2</sub>) as the photocatalyst. The ceramic membranes were synthesized using a sol-gel method, with TiO<sub>2</sub> coatings tailored for precise morphology control. Structural and chemical characterizations conducted through SEM, EDX, and XRD validated the effective incorporation of TiO<sub>2</sub>, which improved membrane hydrophilicity and photocatalytic activity. Performance evaluations indicated that the membranes effectively degraded contaminants, achieving a 99% removal efficiency for Methylene Blue dye in a photocatalytic membrane reactor. The membranes demonstrated selfcleaning and anti-fouling characteristics under UV irradiation, thereby enhancing longevity and operational efficiency. This study emphasizes the viability of cost-effective mineral-based membranes for wastewater treatment, presenting a sustainable and scalable approach for industrial use. The findings establish a basis for future progress in photocatalytic membrane reactors, addressing the balance between cost-effectiveness and high performance in water treatment technologies.

# Epoxy Vitrimers and Composites For High Performance Thermo-Mechanical Applications

Muhammad Faizan Awan

Pak Austria Institute of Science and Technology

Presenting Author: Muhammad Faizan Awan

Abstract: Thermosets and their composites have occupied a key place in the polymeric material industry due to ease of processing, excellent chemical and environmental resistance and high thermal and mechanical performance. But at the same time, they bring a lot waste due to their irreversibility of processing and insoluble nature. Therefore efforts are underway to produce recyclable and degradable thermosets and development of vitrimer polymers is one of them. Vitrimers can be considered as the third category of polymer material beyond traditional thermosets and thermoplastics. An interesting way to produce vitrimer polymer is to customize the chemical structure of the thermoset polymer with covalent adaptive networks before they are produced in their final form. This project also aims to develop a sustainable thermosetting polymer based composite materials bearing high physical and mechanical properties along with the traces of recyclability and re-processability. Thereby, epoxy vitrimer will be designed and prepared as among all thermosets, epoxy resins have occupied 70% of the entire market and are commonly used in adhesives, coatings and composite materials. After the vitrimerization of epoxy resin, its fiber reinforced composites will be developed and will be accompanied by extensive characterisation of mechanical performance of the composites, including quasistatic properties, impact response, and environmental resistance as well assessment of the evolution of properties. Successful completion of this research will provide a composite material system that combines ease of processing, advanced mechanical and thermal properties and the capability to self-heal and be recycled. This will correspond to a significant leap in sustainability of composites that will have the potential to alter industrial practice leading to recyclable advanced composites.

#### **PP43**

# Diclofenac Prodrugs Nanoparticles: An Alternative and Efficient Treatment For Rheumatoid Arthritis?

#### Saadat Hussain

L. E. J. Nanotechnology Center, H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75270, Pakistan.

### Presenting Author: Saadat Hussain

Abstract: We have synthesized new lipidic prodrugs of diclofenac by grafting aliphatic chains (C10, C12, C16 and C18) to diclofenac through an ester bond. Their molecular formulas were confirmed through HR-MS and the formation of ester bond by FTIR and NMR spectroscopy. Nanoparticles of the different prodrugs were successfully formulated using emulsion evaporation method and DSPE-PEG2000 as the only excipient. All nanoparticles were spherical and had a size between 110 and 150 nm, PdI  $\leq 0.2$  and negative Zeta potential values from -30 to -50 mV. In addition, they were stable upon storage at 4 °C up to 30–35 days. The encapsulation efficiency of the prodrug was above 90 % independently of the aliphatic chain length grafted. Nanoparticles did not induce any toxicity on LPS-activated THP-1 cells up to a concentration of 100 µg/mL (equivalent diclofenac) whereas diclofenac sodium salt IC50 was around 20 µg/mL. Following incubation of nanoparticles with LPS-activated THP-1 cells, a dose dependent inhibition of TNF-a was observed comparable to standard diclofenac sodium. Based on in vitro studies representative nanoparticles, Prodrug 3 NPs (C16 aliphatic chain) were selected for further in vitro and in vivo studies. Upon incubation in murine plasma, Prodrug 3 NPs underwent an enzymatic cleavage and almost 70 % of diclofenac was released from nanoparticles in 8 h. In vivo studies on a collagen induced arthritis murine model showed contrasted results: on one hand Prodrug 3 NPs led to a significant decrease of arthritis score and of paw volume compared to PBS after the second injection, on the other hand the third injection induced an important hepatic toxicity with the death of half of the mice from the NP group. To promote the reduction of inflammation while avoiding hepatic toxicity using NPs would require to precisely study the No Observable Adverse Effect Level and the schedule of administration in the future.

# Nanoscale Lipid-Methylprednisolone Conjugates : Effective Anti-Inflammatory, Antioxidant, and Analgesic Agents

### Aqsa Arif

### Hej Research Institute of Chemistry, ICCBS, University of Karachi-75270

#### Presenting Author: Aqsa Arif

Abstract: In this study, we investigated new lipid-drug conjugates (LDCs) of methylprednisolone, a corticosteroid medication, for the potential treatment of inflammatory diseases. lipid-drug conjugates (LDCs), methylprednisolone palmitate The and methylprednisolone palmityl carbonate, were designed by conjugating a C16 aliphatic chain via an ester or carbonate bond, respectively. Their structures were comprehensively characterized using mass spectrometry, nuclear magnetic resonance spectroscopy, and infrared spectroscopy. These LDCs were subsequently formulated into nanoscale particles (NPs) using ethanol injection method. Hydrogenated soybean phosphatidylcholine (HSPC) and tween-80 (Tw-80) served as excipients in the NPs formulation. Characterization via dynamic light scattering and atomic force microscopy confirmed the formation of spherical NPs with a diameter ranging from 100 to 120 nm. The LDCs NPs exhibited excellent stability for about a month, with good polydispersity (below 0.2) and a negative zeta potential between -20 mV to -34 mV. Encapsulation efficiency of the LDCs within the LDCs NPs surpassed 90%, as determined by HPLC analysis. In vitro cytotoxicity studies utilizing LPS-activated THP-1 cells demonstrated no adverse effects associated with LDCs NPs at concentrations up to 100 µg/mL. Furthermore, the NPs effectively retained the anti-inflammatory activity of methylprednisolone, as evidenced by the suppression of IL-1 $\beta$ , TNF- $\alpha$ , and MCP-1 secretion in LPS-stimulated THP-1 cells. The therapeutic potential of these LDCs NPs was further evaluated in rat intervertebral disc-derived nucleus pulposus cells (NPCs). Curative and preventive treatment regimens with the free drug and LDCs NPs 1-2 were employed. Quantitative PCR analysis revealed a significant downregulation of pain and inflammation markers (Substance P and COX-2) along with a concomitant upregulation of antioxidant markers (GPX1, PRDX1, and SOD1) in NPCs treated with both the drug and LDCs NPs 1-2 compared to oxidative stressinduced and control NPCs. Our novel LDCs NPs 1-2 exhibited promising therapeutic potential for treating inflammatory and pain related complications, (including intervertebral disc degeneration). This promise stems from their multifaceted properties, encompassing antiinflammatory, antioxidant, and analgesic effects. Further research is warranted to fully explore LDCs NPs as potential drug candidates in future pre-clinical and clinical trials.

# Synthesis and Evaluation of Folic Acid Functionalized Magnetic Nanoparticles as a Dual System for Electrochemical Detection and Enrichment of Circulating Tumor Cells

Sabeen Iqbal

Bahauddin Zakariya University, Multan

Presenting Author: Sabeen Iqbal

Abstract: Liver cancer is one of the most lethal and aggressive malignancies worldwide. Due to lack of obvious clinical symptoms and tools for sensitive biomarker detection, liver cancer patients often suffer from poor prognosis and diagnosed with disease at an advanced stage. Circulating tumor cells (CTCs) detach from the primary tumor sites, flow in blood cells, and serve as potential biomarkers for the early cancer detection. The efficient, accurate, and rapid detection of CTCs can assist in liquid biopsy and develop devices for prognosis, treatment, and disease monitoring. Herein, a simple, inexpensive and effective dual mode detection system is developed is to identify and capture CTCs by applying synthesized FA-SiO<sub>2</sub>@Fe<sub>3</sub>O<sub>4</sub>. Fe<sub>3</sub>O<sub>4</sub> is synthesized hydrothermally and coated with silica later to develop core shell magnetic material i.e., SiO<sub>2</sub>@Fe<sub>3</sub>O<sub>4</sub>. Fe<sub>3</sub>O<sub>4</sub> that is further functionalized with folic acid (FA) through EDC/NHS chemistry, where FA acts as a recognition element and can bind with CTCs based on the overexpression of folate receptors. The bound CTCs are electrochemically detected through cyclic voltammetry (CV) by applying FA- SiO<sub>2</sub>@Fe<sub>3</sub>O<sub>4</sub>. Fe<sub>3</sub>O<sub>4</sub> coated glassy carbon electrode. A strong redox peak confirms the detection of CTCs in blood samples of cancerous patients. FA- SiO<sub>2</sub>@Fe<sub>3</sub>O<sub>4</sub>. Fe<sub>3</sub>O<sub>4</sub> is also applied to enrich multiple pre-stained cells that are visible under fluorescent microscope. MTT and live/dead assay confirms the biocompatibility of FA-SiO<sub>2</sub>@Fe<sub>3</sub>O<sub>4</sub>. Fe<sub>3</sub>O<sub>4</sub>. The CTCs are enriched and analyzed with improved sensitivity and selectivity by the developed and optimized sensing system.

# Smart MOF Integrated Biopolymeric Hydrogel System : A Novel Strategy for Sustained Anticancer Drug Delivery

Zubdah Ilyas, Usman Liaqat

School of Chemical and Materials Engineering (SCME), National University of Sciences and Technology (NUST), Sector H-12, Islamabad 44000, Pakistan

### Presenting Author: Zubdah Ilyas

Abstract: This study was designed to propose a novel drug delivery system (DDS) on U87 human glioblastoma cell lines using NH2-MIL-88B(Fe) metal organic frameworks as a drug delivery vehicle coated with an optimal ratio of sodium alginate and polyvinyl alcohol (SA/PVA) hydrogel. Initially, the co-precipitation method was used to synthesize NH2-MIL-88B(Fe) MOFs and drug-loaded iron MOF particles while the hydrogel was crosslinked physically and chemically with calcium chloride and glutaraldehyde. Through tensile testing, results showed that SA/PVA thin films had the best mechanical properties at same ratios. XRD, SEM, FTIR, AFM, and DLS analyses were used to confirm the synthesis of fabricated iron MOFs particles, SA/PVA thin films, and SA/PVA thin films incorporated with drug-loaded NH2-MIL-88B(Fe) MOFs particles. According to the AFM and DLS, the average size of the drug-loaded NH2-MIL-88B(Fe) MOF particles was approximately in the range of 1-10 µm. The 5-Fluorouracil release profile was performed by UV-Vis's spectroscopy, and the fabricated SA-PVA@NH2-MIL-88B@5-FU thin films showed controlled release behavior. Additionally, NH2-MIL-88B(Fe) MOFs incorporated in the SA/PVA hydrogel thin films enhanced their stability and showed controlled and prolonged releasing behavior. Furthermore, following a 48-hour incubation period, fabricated DDS's cytotoxicity on human glioblastoma cancer cell lines showed a high viability.

# Enhancing Temperature Regulation on Mars: The Role of Nanorods in Sustainable Habitat Development

Muhammad Bin Javed

University of Sargodha

### Presenting Author: Muhammad Bin Javed

Abstract: Mars' harsh environmental conditions, including extremely low temperatures, pose significant challenges for potential human settlement. Recent advancements in nanotechnology, particularly the use of nanorods, offer innovative solutions to address the thermal limitations of the Martian environment. Nanorods, which have unique thermal properties due to their high surface-area-to-volume ratio, can be utilized to enhance heat absorption and retention on Mars. By integrating carbon-based or metal oxide nanorods into surface materials or habitat structures, it is possible to increase the local temperature by improving infrared absorption and minimizing heat loss. Additionally, nanorods can be employed in the development of thermal management systems for Mars habitats and vehicles, potentially reducing the need for external heating sources. This paper explores the feasibility of utilizing nanorod-enhanced materials for temperature regulation in Martian colonies, evaluating their effectiveness in both passive and active thermal systems. Through simulations and early experimental studies, we demonstrate that nanorod coatings and integration into solar panels could help elevate surface temperatures by several degrees Celsius, providing more hospitable conditions for human life. Ultimately, the integration of nanorod technology could play a crucial role in Mars terraforming efforts and long-term habitability.

# Development of Halal Uni and Bifunctional Bioactive Scaffolds for Hard Tissue Regeneration

Warda Aziz, Maryam Aslam, Adnan Haider, Aqif Anwar Chaudhry, Ather Farooq Khan

Interdisciplinary Research Centre in Biomedical Materials, COMSATS University Islamabad, Lahore campus, Lahore, Pakistan

### Presenting Author: Warda Aziz

Abstract: Treatment of bone loss due to injury or trauma is a critical issue in the field of orthopaedics. Current treatments, such as synthetic bone grafts, are viable options. However, the collagen used for moldability in these grafts is often derived from porcine sources, which poses ethical concerns, particularly in Muslim countries. Additionally, the local unavailability and high cost of these scaffolds hinder their widespread use as an effective treatment. To address these challenges, we synthesized hydroxyapatite and Halal collagen-containing spongy scaffolds. Metal oxide nanoparticles were incorporated into these scaffolds to introduce angiogenic and antibacterial properties. The developed scaffolds were tested for degradation and swelling behaviour. Scanning Electron Microscopy (SEM) was performed to analyse surface morphology. Antibacterial studies were conducted, and the biological activity of the scaffolds was evaluated using cell culture and the (CAM) assay. Furthermore, clinical trials were conducted to assess the in vivo effectiveness of these scaffolds. The results demonstrated that the scaffolds exhibited an optimal degradation rate and high porosity. They also showed good antibacterial activity and were biocompatible. The in vivo trials confirmed the effectiveness of these scaffolds in treating bone injuries. These promising results suggest that this technology has the potential for upscaling, making it a viable solution to address the critical needs of patients.
# Synthesis and Characterization of Cobalt Zinc Oxide (Co-Zno) Nanoparticles By Co-Precipitation Method For Energy Storage Application

Maria Khattak and Asma wali

Presentation

### Presenting Author: Asma wali

Abstract: Cobalt-Zinc Oxide nanoparticles (Zn 1-x Co x O) (x=0.03) were created through a budget-friendly, environmentally friendly process called co-precipitation. This involved mixing Cobalt nitrate hexahydrate and Zinc nitrate hexahydrate as starting materials. The XRD study reveals that the Co-ZnO nanoparticles are composed of hexagonally shaped wurtzites, and that the diffraction peaks are shifted to higher angles, indicating the characteristic influence of the Co, whose ionic radius is smaller than that of its host cation. The crystallite size has been calculated using the Scherrer formula. Additionally, the surface morphology of the product and its elemental analysis have been characterized using scanning electron microscopy (SEM) and energy dispersive spectra(EDX). Fourier Transform Infrared (FTIR) spectroscopy is also have been performed. The electrochemical performance of the synthesized material was studied by cyclic voltammetry (CV) and electrochemical impedance-spectroscopy (EIS) techniques in 0.5 M sulfuric acid (H<sub>2</sub>SO<sub>4</sub>) electrolyte under a potential window range of -2.5 to 3.0 V. The specific capacitance of pure Co-ZnO calculated from the CV curve were 187.8, 0.62 and 0.39 Fg<sup>-1</sup> respectively at a scan rate of 10 mVs<sup>-1</sup>. Tests with electrochemistry revealed the materials suitability as a high-performance electrode for energy storage applications, showing excellent specific capacitance. This study supports the goals of sustainable development by offering a cost- efficient and eco-friendly method for energy storage. Crucially, both the process of making the material and the material itself are non-toxic to the environment or the climate, making it a viable and hopeful solution for tackling worldwide energy issues.

## Hydrothermal Synthesis and Photocatalytic Performance of Pure and Ce-Doped CdS Quantum Dots for Solar-Driven Applications

Fareeha Nazar, Hafsa Bibi, Attaullah Shah, Muhammad Asim Rasheed

Physics Department, Pakistan Institute of Engineering and Applied Sciences, Nailor Islamabad

Presenting Author: Fareeha Nazar

Abstract: Cadmium sulfide (CdS) quantum dots (QDs) are widely studied for photocatalytic applications due to their excellent optical properties and ability to harness solar energy. However, challenges such as rapid charge recombination limit their efficiency. Rare-earth doping, particularly with cerium (Ce), has emerged as a promising strategy to enhance charge separation and improve photocatalytic performance. Objectives: This study aims to synthesize and investigate the structural, optical, and photocatalytic properties of undoped and Ce-doped CdS QDs to evaluate the effect of Ce doping on their efficiency in solar-driven photocatalysis. Methods: CdS QDs were synthesized using a hydrothermal method, with cerium incorporated as a dopant. Structural characterization was performed using X-ray diffraction (XRD) to confirm phase purity. Raman spectroscopy was employed to analyze vibrational modes and assess crystallinity. Optical properties were studied via UV-Vis spectroscopy and photoluminescence (PL) to determine bandgap modifications and charge carrier dynamics. The photocatalytic performance was assessed by monitoring the degradation of organic pollutants under simulated solar irradiation. Results: Ce-doped CdS QDs exhibited red shifts in absorption, reduced bandgap energy, and enhanced charge carrier separation compared to undoped CdS. Photocatalytic experiments demonstrated significantly improved degradation rates for Cedoped CdS, attributed to reduced electron-hole recombination and improved charge transport. These findings highlight the potential of Ce-doped CdS QDs for sustainable photocatalytic applications.

### Sonochemically Synthesized 2D Silver based MOF for Energy Storage Devices

Maham Saeed, Shahzad Sharif\*, Javed Hussain Shah, Tayyba Tur Rehman Afzal, Muhammad Shahbaza

### Government College University, Lahore

### Presenting Author: Dr. Shahzad Sharif

Abstract: The rising demand for advanced energy storage devices having superior energy and power density has propelled the development of hybrid supercapacitors by integrating capacitive and battery-grade materials in a single device. This drives expedition is ongoing research for the development of advanced materials. In this regard, metal-organic frameworks (MOF) comprising metal nodes and organic ligands containing nitrogen atom evolved as leading candidates for their customized and extraordinary features. Here, we have synthesized copper-based 1D conductive MOF from 2,6-pyridinedicarboxylic acid (PDA) and structurally characterized by using single-crystal X-ray diffraction, FT-IR, TGA and elemental analyzer techniques. PDA ligands are connected by copper ions with 1D  $\pi$ -d conjugated layers. The presence of oxygen and nitrogen heteroatoms on PDA promotes high surface area, porosity as well as facilitates more electrolyte-ions to active sites, resulting in increased redox potential and charge storage responsible for enhanced conductivity and stable framework. Detailed electrochemical performance was investigated through a three-electrode assembly using CV, GCD, and EIS techniques. Analysis of the material exhibited characteristics of advanced battery-grade material. Based on its inherent electrochemical features, it was practically validated by integrating Cu-PDA-MOF (battery-grade) as positive electrode and activated carbon (capacitive-grade) as negative electrode in two-electrode set up. The hybrid device possessed extraordinary electrochemical features with specific capacity of 160.59 C/g, energy density of 31.23 Wh/kg, and power density of 1400 W/kg. Remarkably, the hybrid material showed 99.8% cyclic stability even after 5000 GCD cycles. These advanced electrochemical features underscore Cu-PDA-MOF as a highly attractive material for futuristic energy storage devices. High energy density and power density with extraordinary stability make Ag-MOF electrode a promising candidate for futuristic hybrid supercapacitor devices and rechargeable aqueous zinc batteries (ZBs).

## Electrochemical Investigation of Copper 1D Conductive Polymer For Hybrid Supercapacitor Applications

Javed Hussain Shah, Muhammad Shahbaz, Maham Saeed, Ayesha Shahzad, Sidra Farid, Sundas Shahzad, Shabbir Muhammad, Shahzad Sharif

Materials Chemistry Laboratory, Department of Chemistry, Government College University Lahore, 54000, Pakistan, Department of Chemistry, College of Science, King Khalid University, P,O. Box 9004, Abha 61413, Saudi Arabia

#### Presenting Author: Maham Saeed

Abstract: The rising demand for advanced energy storage devices having superior energy and power density has propelled the development of hybrid supercapacitors by integrating capacitive and battery-grade materials in a single device. This drives expedition is ongoing research for the development of advanced materials. In this regard, metal-organic frameworks (MOF) comprising metal nodes and organic ligands containing nitrogen atom evolved as leading candidates for their customized and extraordinary features. Here, we have synthesized copper-based 1D conductive MOF from 2,6-pyridinedicarboxylic acid (PDA) and structurally characterized by using singlecrystal X-ray diffraction, FT-IR, TGA and elemental analyzer techniques. PDA ligands are connected by copper ions with 1D  $\pi$ -d conjugated layers. The presence of oxygen and nitrogen heteroatoms in PDA promotes high surface area, porosity as well as facilitates more electrolyte-ions interclation to active sites, resulting in increased redox potential and charge storage responsible for enhanced conductivity and stable framework. Detailed electrochemical performance was investigated through a three-electrode assembly using CV, GCD, and EIS techniques. Analysis of the material exhibited characteristics of advanced battery-grade material. Based on its inherent electrochemical features, it was practically validated by integrating Cu-PDA-MOF (battery-grade) as positive electrode and activated carbon (capacitive-grade) as negative electrode in two-electrode set up. The hybrid device possessed extraordinary electrochemical features with specific capacity of 160.59C/g, energy density of 31.23 Wh/kg, and power density of 1400 W/kg. Remarkably, the hybrid device showed 99.8 % cyclic stability even after 5000 GCD cycles. These advanced electrochemical features underscore Cu-PDA-MOF as a highly attractive material for futuristic energy storage devices.

## Influence of Marine Pollution on Corrosion Behavior of Ship Steels and Cupronickel Alloys in the Coastal Seawaters of Pakistan

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Abstract: Corrosion in metals exposed to seawater is immensely affected by the variations in the composition of seawater, especially by the amalgamation of pollutant factors nearby the harbours and coasts closed to industrial sites. Marine pollution is one among the most influential factors that not only disturbs the ecological system in coastal regions but it also contributes towards the aggravated rate of corrosion of marine assets and associated infrastructure. Coastal seawaters of Pakistan especially near the coast of Karachi are flooded with numerous type of domestic, industrial and agricultural wastages, which immensely transforms the chemical characteristics of coastal seawater in this region. This in turn inflict additional costs on upkeep, operation and maintenance of offshore infrastructure shipping industry in particular. This study investigates the corrosion behaviour of steel and cupronickel alloys in pollutant-rich seawater compositions along Karachi harbour, and compares them with the corrosion losses resulted for similar material exposed in the clean and natural seawater sites. The deposited corrosion products have also been characterized using various analytical techniques, to develop a relationship between corrosion rates and characteristics of corrosion deposits collected from two different exposure conditions. Numerous inferences between the pollutant factors in seawater and the rate of corrosion process have been developed on the basis of the corrosion tests conducted for extended durations.

# Optimizing PV Panel Cooling Using Jeffrey Nanofluids with Nonlinear Thermal Radiation

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Abstract: Electricity generation through solar energy/heat has the potential to meet the growing energy demands of the world. The efficiency of these systems is greatly effected by varying temperatures and the performance of photovoltaic systems decreases with increase in operating temperature above 25 °C. In this study a prototype thermal management system involving nanofluid is proposed for the photovoltaic thermal solar system. Tube heat exchanger filled with nanofluid will act as a coolant and improve heat dissipation and enhancing overall panel efficiency. The mathematical model incorporate incompressible Jeffrey nanofluid flow in an inclined tube heat exchanger positioned at the rare of PV panel. The flow is under the influence of buoyancy forces and the nanoparticles are uniformly distributed in the basefluid. Non-linear thermal radiations are considered through Rosseland's approximations. The governing partial differential equations (PDEs) are formulated based on conservation laws. Suitable similarity transformations are employed to transform the governing PDEs in ordinary differential equation (ODEs) and then solved numerically using MATLAB's BVP4C solver. The Copper nanoparticles are assumed to be uniformly distributed in the Kerosene basefluid. The system is analyzed and the numerical solutions are presented in the form of graphs and tables and discussed for the various values of the governing parameters. Namely inclination angle, nanoparticle concentration, Prandtl number and radiation parameter.

## Impact of Nonlinear Thermal Radiation for Flow in an Inclined Absorber Pipe in PV Solar Thermal Systems

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Abstract: This work proposed a prototype model for the flow and heat transfer of ternary hybrid Casson nanofluid in an inclined absorber pipe underneath the photovoltaic thermal (PVT) system. The PVT system combines PV panels and thermal collectors for generating electricity and heat simultaneously. The efficiency of the system is greatly affected by the temperature variations. Therefore, this particularly focuses on the impact of nonlinear thermal radiation on the performance of photovoltaic thermal systems. The nanoparticles are uniformly distributed in the base fluid, and the boundaries of the pipe are considered to be convective. The governing partial differential equations (PDEs) are derived from conservation laws, incorporating the nonlinear radiation terms in the form of qrad =  $\sigma$  (T4 – T4  $\infty$ ), where T is the temperature and  $\sigma$  is the Stefan-Boltzmann constant. The governing partial differential equations are numerically solved using MATLAB's byp4c solver. The effect of key parameters on the flow and heat transfer characteristics are examined. The results signify the impact of nonlinear thermal radiation in improving heat dissipation and overall efficiency of the system.

















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