

**2 Days International e-Conference on**

**"Advanced Materials: Bridging Physics,  
Chemistry, Biosciences and  
Computational Modelling  
(AMBPC-2026)"**

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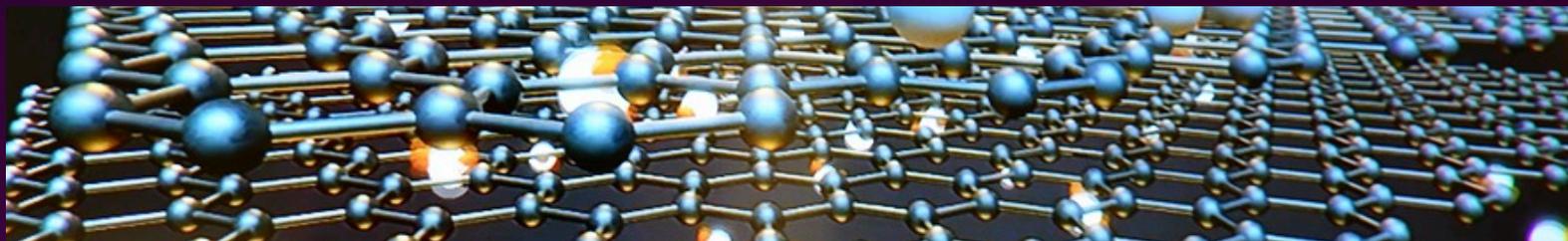
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### Valedictory Speech

Development of Optical Elements from the Uniaxial Organic Crystals



**Dr. Muthu Senthil Pandian**  
Ph.D. FASCh.

**Research Scientist (Grade-III)  
Photovoltaic Devices Laboratory  
SSN Research Centre, SSN Institutions  
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### SPEAKERS

### Plenary Talk- I

Emerging Nonlinear Optical Materials for High-Performance Photonics



**Dr. Vinitha G**  
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VIT, Chennai,  
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### Plenary Talk- II

Synthesis of Nanocomposites and exploring their activities



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**Department of Environmental Engineering and Management, Chaoyang University of Technology  
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## 1. Bridging the Realms of Mathematics and Chemistry: A Comprehensive Theoretical and Applied Study of Degree-Based Topological Indices

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### ABSTRACT

Degree-based topological indices are important tools in mathematical chemistry for measuring molecular structure and predicting physicochemical properties. This study offers a detailed comparison of three key degree-based indices: the first and second Zagreb indices ( $M_1$  and  $M_2$ ) the Randic index ( $R$ ), and the Harmonic index ( $H$ ), across various types of graphs. Through careful mathematical work and computational testing, we establish clear expressions and relationships among these indices for path, cycle, complete, and regular graphs. The results show that for all regular graphs,  $R(G)$  equals  $H(G)$ , which suggests a structural overlap in highly symmetric molecular systems. On the other hand, for trees and irregular graphs, different behavioural patterns appear, with the Harmonic index often displaying stronger links to physical properties like boiling points and molecular strain energy. Additionally, we present new bounds and inequalities that define the relative sizes of these indices, offering greater insight into their structural sensitivity. These findings lay a theoretical foundation for effectively choosing and using degree-based descriptors in QSPR/QSAR modelling, enhancing predictive reliability and limiting redundancy in chemical graph theory.

*Keywords: Degree-Based Indices, Zagreb Indices, Randic Index, Harmonic Index, Topological Descriptors, Chemical Graph Theory, QSPR/QSAR, Regular Graphs, Molecular Structure, Structure–Property Relationships*

## 2. Multifaceted Exploration of p-Toluic Acid Single Crystals: Structure, Optics, and Nonlinear Photonic Potential

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### ABSTRACT

This research explores the structural, optical, mechanical, and nonlinear optical properties of p-toluic acid single crystals obtained by slow evaporation. SXRD and PXRD ascertained phase purity, FTIR determined functional groups, and UV–Vis spectroscopy ascertained transparency and band gap. SEM, LDT, contact angle, chemical etching, and microhardness tests evaluated morphology, stability, wettability, defects, and strength. Z-scan measurements established third-order susceptibility and nonlinear refractive index. Hirshfeld and 2D fingerprint investigations revealed H···H (38.9%), O···H/H···O (31.8%), and C···C (8.5%) contacts, i.e., hydrogen bonding and  $\pi$ – $\pi$  stacking. Energy framework calculations presented major dispersion forces ( $E_{dis} = -34.8$  kJ/mol at 3.62 Å) supplemented by electrostatics and polarization effects, improving mechanical strength and nonlinear optical activity.

*Keywords: Organic materials, Hardness, Nonlinear optical materials, Laser damage threshold, Self-defocusing.*

## 2. The Impact of Pollutants on Biological Food Chain System: A Mathematical Approach

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### ABSTRACT

A biological mathematical food chain model is considered to study the impact of pollutants on prey predator food chain populations. In the mathematical model it assumed that the population of prey releases harmful toxins for its protection. Logistically the prey population increases and for the interactions between populations Holling type 2 response considered. Discussed all the equilibrium points and studied the conditions of stability. It has been observed that when prey releases pollutants or toxicants then the predator populations reduce. Finally, analytical results are satisfied with numerical simulations. For simulations, MATLAB software is used

*Keywords: MATLAB, Mathematical Model, Food chain*

### **3. Bridging Physics, Chemistry, Biosciences and Computational Modelling**

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#### **ABSTRACT**

The development of advanced materials has become a central scientific theme owing to their transformative potential across engineering, medicine, energy, and environmental applications. This interdisciplinary research explores the synthesis, characterization, and application of novel advanced materials by integrating principles from physics, chemistry, biosciences, and computational modelling. The study aimed to bridge disciplinary boundaries to establish a unified framework for understanding material behavior at multiple scales—from atomic interactions to macroscopic properties. A dataset of 200 samples, encompassing experimental measurements and simulation results, was acquired across various material classes including nanocomposites, biomimetic polymers, and quantum dot systems. Advanced characterization techniques (e.g., spectroscopy, electron microscopy) provided insights into structural and chemical features, while computational modelling (density functional theory, molecular dynamics) guided predictions of performance and mechanisms. Multivariate statistical analysis and machine learning protocols were used to interpret correlations between compositional variables and functional outcomes. Key findings reveal that specific atomic configurations and surface chemistries strongly influence mechanical strength, electronic properties, and biocompatibility. The integration of computational insights significantly reduced experimental burdens and enabled identification of optimal material designs with enhanced performance metrics. However, challenges in scaling predictive models and ensuring reproducibility across diverse material systems were identified as key limitations. Future work is recommended to develop standardized data sharing protocols and hybrid experimental-computational workflows. This research consolidates multidisciplinary strategies as a foundation for next-generation material design and underscores the importance of integrative approaches in advancing fundamental and applied scientific knowledge.

*Keywords: Advanced materials, interdisciplinary research, computational modelling, biosciences, materials characterization, machine learning, multiscale analysis.*

## **5. Evaluating the Environmental Benefits of Biodegradable and Recyclable Waste Materials: Air Pollution Reduction in Glass, Plastic, and Metals**

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### **ABSTRACT**

Effective waste management practices are critical for mitigating environmental impact and promoting sustainability. This paper explores the role of biodegradable waste in addressing these challenges and presents comparative data on the reduction of air pollutants associated with various waste materials. The analysis reveals that biodegradable waste can significantly lower emissions compared to traditional materials. Specifically, glass waste results in 18% to 30% less air pollution, while plastic waste can reduce emissions by up to 66%. In contrast, iron cans contribute to 70% to 86% less air pollution, and aluminum cans are associated with a dramatic 95% reduction in air pollutants. These findings underscore the environmental benefits of transitioning towards more sustainable waste management practices and highlight the potential for biodegradable and recyclable materials to play a crucial role in minimizing air pollution and enhancing ecological sustainability.

*Keywords: - Air Pollution Reduction, Recycling Efficiency, Biodegradable Materials, Waste Management, Glass Recycling, Plastic Waste, Metal Cans.*

## 6. Inventory Optimization for Sustainable Advanced Material Supply Chains

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### ABSTRACT

The rapid adoption of advanced materials in modern manufacturing and biomedical industries has increased the complexity of inventory management due to high production costs, specialized storage requirements, and sustainability concerns. Traditional inventory models often fail to adequately capture the environmental and operational challenges associated with advanced material supply chains. This paper presents an inventory optimization framework for sustainable advanced material supply chains, integrating economic, environmental, and operational considerations. The proposed model incorporates sustainability-oriented factors such as carbon emissions, resource utilization, waste reduction, and material lifecycle characteristics alongside classical inventory costs. Advanced materials with unique physical and chemical properties are considered under demand uncertainty and limited storage conditions. Computational modelling techniques are employed to determine optimal inventory policies that balance cost efficiency with environmental performance. The results demonstrate that incorporating sustainability constraints into inventory decision-making leads to significant improvements in resource efficiency and emission reduction without compromising service levels. The proposed framework offers a practical decision-support tool for managing advanced material inventories and contributes to the development of sustainable and resilient material supply chains.

*Keywords: resource utilization, environment, supply chains*

## 7. Fabrication and Characterization of Citric Acid–Cross-linked CMC–PEG Hydrogel Films for Controlled Drug Release

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### ABSTRACT

Hydrogels are three-dimensional polymeric networks capable of absorbing large amounts of water while maintaining their structure, making them promising for biomedical uses, including drug delivery and wound healing. In this study, citric acid-crosslinked carboxymethylcellulose (CMC) and polyethylene glycol (PEG) hydrogel films were developed to enhance the solubility and provide controlled release of poorly soluble drugs, specifically ketoconazole (KTZ). The hydrogels were synthesized via esterification, where citric acid formed crosslinks between hydroxyl groups of CMC and PEG. The resulting films were characterized using Thermogravimetric Analysis (TGA), Scanning Electron Microscopy (SEM), and Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR), confirming improved thermal stability, flexibility, and crosslinking efficiency compared to pure CMC hydrogels. Swelling behavior and drug-loading capacity were evaluated, with formulation D/CP3 showing the highest swelling ratio ( $12.4 \pm 0.3$  g/g in PBS) and sustained drug release, making it the most promising candidate. Antifungal efficacy was demonstrated against *Saccharomyces boulardii*, with a clear zone of inhibition observed, confirming the bioactivity of the KTZ-loaded hydrogel. Overall, the CMC-PEG hydrogel films, particularly D/CP3, offer a biocompatible, cost-effective, and efficient platform for the controlled delivery of hydrophobic drugs. Further in vivo studies are recommended to validate these findings for clinical applications.

*Keywords: Carboxymethylcellulose, Polyethylene Glycol, Citric Acid, Hydrogel Films, ketoconazole, Controlled Drug Release*

## 8. Neutrosophic Multi-Criteria Decision-Making for Eco-Conscious Material Selection

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### ABSTRACT

The growing demand for sustainable development has intensified the need for systematic selection of eco-conscious materials that balance environmental, technical, and economic considerations. Material selection in sustainable engineering is inherently complex due to the presence of multiple conflicting criteria and high levels of uncertainty, imprecision, and indeterminacy in expert assessments. This paper presents a Neutrosophic Multi-Criteria Decision-Making (MCDM) framework for the evaluation and selection of eco-conscious materials. The proposed approach employs neutrosophic sets to effectively model truth, indeterminacy, and falsity degrees associated with sustainability criteria such as environmental impact, resource efficiency, recyclability, mechanical performance, cost effectiveness, and lifecycle considerations. By integrating expert knowledge within a neutrosophic decision environment, the framework enables robust aggregation and ranking of alternative materials under uncertain and incomplete information. The results demonstrate that the neutrosophic MCDM approach enhances decision reliability and transparency compared to conventional fuzzy or crisp methods. The proposed methodology provides an effective decision-support tool for eco-conscious material selection and contributes to sustainable material design by bridging advanced materials, environmental sciences, and computational decision modelling.

*Keywords: Neutrosophy, Sustainability, Eco-Conscious Material*

## 9. Efficiency of 1,3-Dibromo propane as an ATRP initiator for synthesis of bifunctional polystyrene

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### ABSTRACT

A new atom transfers radical polymerization (ATRP) initiator, namely 1, 3-dibromopropane (1,3-DBP), was applied successfully for the synthesis of high molecular weight polystyrene, a commercially available and inexpensive compared to conventional ATRP initiators. The ATRP was conducted with mole ratio of [Styrene]:[1,3-DBP]:[CuBr]:[PMDETA]=500:1:1:2 in bulk and solution as well for the first time. Well defined bromine-end-functionalized polystyrenes with narrow molecular weight distribution (1.10-1.35) were synthesized using ATRP by varying the concentration of monomer vs. initiator. The presence of bromine at the polystyrene chain end was confirmed using spectroscopic techniques such as Fourier transform infrared (FT-IR), Nuclear magnetic resonance (NMR) and Energy-dispersive X-ray (EDX). The nearness was observed between calculated and experimental molecular weights at higher conversion. The initiator efficiency (f) was found between 0.5-0.8 in some cases. The molecular weight distribution was narrow compared to free radical initiators and follows the linearity with the progress of the reaction. Furthermore, 1, 3-DBP was studied for the dependency on copper concentration and it was reduced to 10% of its initial concentration.

*Keywords: FTIR, ATRP, Styrene, atom*

## 10. Collisional interactions of Multicomponent Component Non linear system via Painlevé truncation for optical fibre communication

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### ABSTRACT

The (2+1) - dimensional NLSE system constitutes an important class of multicomponent nonlinear evolution equations capable of describing complex wave interactions in higher-dimensional media. A thorough analytical study of this system is undertaken using the truncated Painlevé approach which serves as a powerful and systematic tool for probing integrability while simultaneously enabling the construction of exact solutions. By performing a truncated Laurent series expansion of the dependent variables, a general solution framework involving arbitrary functions is obtained. This formulation provides substantial freedom in tailoring solution profiles and reveals the inherent richness of the system's nonlinear dynamics. By selecting appropriate forms of the arbitrary functions a wide variety of localized coherent structures are generated, including dromions, multi-rogue wave configurations and lump solitons. These solutions exhibit pronounced spatiotemporal localization and intricate evolution patterns arising from strong coupling among the multiple wave components. The coexistence and transformation of different localized modes highlight the complex energy redistribution mechanisms present in higher-dimensional multicomponent systems. The interaction dynamics of these localized excitations are analyzed in detail, demonstrating elastic collision behavior with complete preservation of amplitude, profile and propagation characteristics after interaction. Such robustness confirms the integrable nature of the system and underscores the stability of the obtained solutions. The present study not only illustrates the effectiveness of the truncated Painlevé approach in handling higher-component nonlinear systems but also contributes to a deeper understanding of resonant interactions, energy localization and coherent structure formation in multidimensional nonlinear wave dynamics. These findings may be relevant to a range of physical settings including optical fiber communication, Bose–Einstein condensates, plasma physics and fluid dynamical systems.

*Keywords: Truncated Painlevé approach, Dromion, Lump, Rogue wave.*

## 11. Physico Chemical characterization studies of MgO-PVA nano composite, CaO-MgO-PVA nanocomposite and its bio medical application

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### ABSTRACT

The jujube tree, also known as “Ziziphus jujube”, is a valuable and delicious fruit that has been consumed for thousands of years around the world. It is rich in vitamins, minerals and antioxidants, making it a popular choice in various fields. Objective for this investigation was green synthesis of MgO-PVA nano composite and CaO-MgO-PVA nano composite were prepared by using jujube fruit, characterization studies and their applications. MgO-PVA and CaO-MgO-PVA nanocomposite were prepared using a green method that is safe for the environment with the help of jujube fruit. The UV- visible spectrophotometer was used to record the UV-visible spectra of MgO-PVA, CaO-MgO-PVA nanocomposite powder, in the wavelength range between 270-500nm. The characteristic absorption band appeared at 274 nm, 271 nm, 330 nm Moreover, FTIR was used to determine the functional groups, present in the MgO-PVA, CaO- MgO-PVA nanocomposite. TEM results showed the spherical size and crystalline nature of MgO-PVA nanocomposite. MgO-PVA and CaO-MgO-PVA nanocomposite were screened for anti-microbial activity.

*Keywords: Jujube fruit, UV visible spectrophotometer, TEM studies, MgO-PVA nanocomposite, CaO-MgO-PVA nanocomposite*

## 12. Design and Evaluate Novel Sodium/Glucose Co-transporter 2 Inhibitors for Efficacious Anti-Diabetic Pharmacotherapy

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### ABSTRACT

The global rise in type 2 diabetes mellitus (T2DM) continues to impose a significant burden due to its association with long-term microvascular and macrovascular complications affecting the cardiovascular, renal, and nervous systems. Sodium–glucose cotransporter-2 (SGLT-2) inhibitors have emerged as a promising class of antidiabetic drugs. In addition to glycemic control, these agents have demonstrated notable cardiovascular and renal protective effects. In this context, the present study employs an integrated computational drug discovery approach to design and evaluate novel SGLT-2 inhibitors with enhanced antidiabetic efficacy and antioxidant potential. A comprehensive in-silico workflow was implemented, encompassing pharmacophore modeling, virtual screening, absorption, distribution, metabolism, and excretion (ADME) prediction, molecular docking, molecular dynamics (MD) simulations, and density functional theory (DFT) calculations. From extensive virtual screening, two lead compounds—ZINC77285189 and ZINC59047505—were identified as potential SGLT-2 inhibitors with favorable pharmacokinetic and drug-likeness profiles. The stability of the ligand–protein complexes was further validated through MD simulations and MM-GBSA free energy calculations, confirming persistent interactions and structural integrity throughout the simulation. DFT analysis provided insights into the electronic properties of the leads, revealing high electron affinity and electrophilicity. Notably, ZINC77285189 exhibited the smallest HOMO–LUMO band gap, indicative of superior electronic reactivity and enhanced antioxidant potential.

Overall, this study highlights the effectiveness of computational drug design strategies in identifying potent, stable, and pharmacokinetically viable next-generation SGLT-2 inhibitors, offering a strong foundation for subsequent experimental and clinical validation.

*Keywords: SGLT-2 inhibitors, ADME, Docking, MD simulation, DFT studies*

### 13. Pathways and Persistence of Microplastics in Food and Water-A Hidden Threat to Human Health

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#### ABSTRACT

Plastic has become ubiquitous in the daily life of human beings. Microplastics are tiny plastic particles less than 5 mm in size, invisible to the naked eye and are now detected in soil, air, rivers and oceans. Further they are intentionally added in food, cosmetics, which lead to constant human exposure and are likely to be found in the blood, lungs, placenta, breast milk. This widespread presence makes microplastic a dominant environmental and health concern. This study reviews their pathways from industrial and domestic sources into food and water, with a specific focus on contamination. To assess public awareness, a survey was conducted among 100 young Omani adults, predominantly university students. The results revealed a high level of understanding regarding sources (e.g., plastic manufacturing, fishing gear), exposure routes (primarily through bottled water and seafood), and perceived health risks, with cancer and respiratory issues ranked highest. 66% of participants recognized microplastics as a continuing toxic threat to future generations. However, a significant gap exists between students and the public awareness of microplastics. This study recommends implementing a phased ban on non-essential microplastics and single-use plastics, launching nationwide awareness campaigns, investing in local research and biodegradable alternatives, and enforcing extended producer responsibility to mitigate this crisis and protect public health and the environment in Oman.

*Keywords: Food, water, plastics, omani adults*

## **14. Neuronal Heterogeneity Within the Anterior Hypothalamus (Ah) in Wistar Rat**

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### **ABSTRACT**

The anterior hypothalamus (AH) is situated in front of hypothalamus, extends from optic chiasm towards the median eminence forming the rostral part just above the third ventricle. It is the most prominent field of hypothalamus as it contains major key nuclei including suprachiasmatic nucleus (SCN), supraoptic nucleus (SON), paraventricular nucleus (PVN) and preoptic nucleus (PON) which are responsible for social and sexual behaviors. Neurons are the structural and functional unit of the nervous system. They have three distinct parts including a cell body or soma, axon (specialized projections) and dendrites for impulse transmission. The neuronal morphology and diversity in AH of wistar rats have been studied using Golgi-Colonnier technique. Based on axonal projection, soma shape, size and dendritic field extent Multipolar, Pyramidal, Stellate, Unipolar, Bipolar and Glial neurons have been identified. This finding suggests that the diverse structural morphology in neurons contribute to the better and versatile functionality of AH in rat.

*Keywords: Anterior Hypothalamus, Neuron, Heterogeneity, Soma.*

## 14. Recent Advances and Challenges in Membrane Distillation for Water Desalination and Wastewater Treatment

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### ABSTRACT

Membrane distillation (MD) is a promising thermally-driven separation process that uses hydrophobic membranes to separate water vapor from saline or contaminated water. Unlike conventional reverse osmosis (RO), MD can operate at low temperatures and utilize waste heat or solar energy, making it suitable for sustainable desalination. Despite its potential, challenges such as membrane fouling, scaling, wetting, and energy efficiency still limit large-scale application. A review that synthesizes recent progress, innovations, and challenges would be highly valuable to the scientific community.

*Keywords: membrane distillation, wastewater treatment, desalination, industrial effluent, brine concentration*

## 16. Isolation Of Amylase Producing Bacteria from Soil and Its Efficacy In Removing Chocolate Stain

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### ABSTRACT

Amylase enzyme use has been extensive in different industrial sectors. The present study is an attempt to extract amylase producing bacteria and to evaluate their destaining properties for detergent additive. The isolation of amylase enzyme producing bacteria was carried out from soil sample collected from kitchen waste dump sites of surrounding regions of Kochi, Kerala. Enzyme production was identified by formation of halos around the colonies indicating degradation of starch using amylase. The most potent amylolytic bacterial strains were Isolate 2 and isolate 4 which displayed an enzymatic index of 2.32 and 2.75 respectively. The enzymatic index is generally proportional to amylase production so the same were selected for further evaluation. Morphological and Molecular identification revealed the identity of the organism as *Bacillus amyloliquefaciens* (Isolate 2) and *Bacillus licheniformis* (Isolate 4). Characterization of the crude amylase enzyme revealed that the optimum temperature of the enzyme was 75°C while the optimum pH was 7. The optimum incubation time for amylase production was found to be 48 hours for both the isolates. The application of the extracted enzyme from the isolates as destaining agents was studied using the removal of chocolate stain. Treatment with extracted enzyme as well as detergent (tween 80) alone did not promote complete removal of the stains. However, an increase in amylolytic activity was recorded on combination with detergent. These bacteria can be used for amylase production and applied locally and nationally in agriculture, food processing and textile industries in the future. Thus, this will reduce the cost of industrial enzyme import from other countries, offer sustainability of local enzyme production and enhance the economy of the nation.

*Keywords: Amylase, Bacillus amyloliquefaciens, Amylolytic, Bacillus licheniformis, Destaining agents, tween 80*

## 17. Role of Biosciences in Environmental Protection and Ecological Balance

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### ABSTRACT

Environmental protection has become a major concern worldwide due to increasing pressure from industrial growth, urbanization, intensive farming practices, and overuse of natural resources. These activities have resulted in pollution, degradation of ecosystems, loss of biodiversity, and disturbance of ecological balance. Biosciences offer valuable scientific insights into understanding environmental problems and provide sustainable, nature-based solutions for their management. Various branches of biosciences, including ecology, microbiology, environmental biology, biotechnology, and conservation science, play an important role in pollution control, ecosystem restoration, and biodiversity conservation. Biological approaches such as bioremediation, bioindicators, sustainable agricultural practices, and biological pest management help reduce environmental damage while maintaining ecosystem stability. This paper presents a comprehensive review of recent scientific studies to highlight the contribution of biosciences in environmental protection and the maintenance of ecological balance. The study emphasizes that the effective application of bioscientific knowledge, along with supportive environmental policies, is essential for achieving long-term sustainability and ecological harmony.

*Keywords:*

*Biosciences; Environmental Protection; Ecological Balance; Sustainability; Biodiversity Conservation; Bioremediation; Bioindicators; Ecosystem Restoration*

## 18. Phase and Magnetic Evolution in Europium-Doped Lanthanum Ferrite Perovskite Nanoferrites

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### ABSTRACT

This work explores how europium substitution influences the phase behaviour and magnetic response of Lanthanum Ferrites (LaFeO<sub>3</sub>) perovskite nanoferrites synthesized through the solution combustion route. X-ray diffraction (XRD) confirms the formation of a single-phase perovskite structure, and the observed reduction in lattice constants demonstrates that Eu ions are successfully incorporated into the LaFeO<sub>3</sub> lattice. Field emission scanning electron microscopy (FESEM) shows a uniform grain arrangement, together with an increase in porosity at higher Eu contents. Energy-dispersive X-ray analysis (EDX) confirms the expected elemental composition in both undoped and Eu-doped samples, indicating high material purity. High-resolution transmission electron microscopy (HRTEM) further reveals the nanocrystalline nature of the powders and displays distinct lattice fringes, reflecting good crystallinity and allowing estimation of interplanar spacing and particle dimensions. Magnetic measurements carried out using a SQUID magnetometer show a progressive modification in magnetic behaviour with increasing Eu concentration, including higher magnetic moments and coercivity. These findings demonstrate that europium doping provides an effective route to tailoring the phase stability and magnetic functionality of LaFeO<sub>3</sub> nanoferrites, making them promising candidates for future spintronic and magnetic data-storage applications.

*Keywords: LaFeO<sub>3</sub> nanoferrites; Europium doping; Phase evolution; Magnetic properties; Solution combustion synthesis*

## 19. Design and Development of a Solar Panel Efficiency Testing Module

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### ABSTRACT

This paper details the design and development of a portable, cost-effective diagnostic module for real-time monitoring of solar panel health via integrated thermal analysis. Traditional inspection methods often require expensive industrial imaging; this research proposes a non-invasive alternative utilizing a low-power ESP32-CAM microcontroller integrated with a high-precision MLX90614 infrared temperature sensor. This configuration enables non-contact detection of localized hotspots—a key indicator of photovoltaic (PV) cell degradation and electrical underperformance. To ensure field utility, the module incorporates an 8GB micro SD card for offline data logging and is powered by a dual 18650 Li-Ion battery system, providing high autonomy for remote inspections. The software architecture, developed in the Arduino environment, employs a threshold-based logic to categorize panel status as "Good" or "Faulty" based on thermal limits between 45°C and 55°C. Experimental results validated the system's efficacy, successfully identifying panel faults invisible to the naked eye. By providing an accessible, scalable tool for early fault detection, this research contributes to extending the operational lifespan and efficiency of solar infrastructure.

*Keywords: Photovoltaic (PV) Systems, Solar Panel Monitoring, MLX90614 Sensor*

## **20. DFT Based Molecular Geometry, Electronic Structure, and Electrostatic Potential Analysis of Heptadecane from *Entada pursaetha* Tuber Extract**

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### **ABSTRACT**

*Entada pursaetha* tuber extract is an ethnomedicinally important natural source traditionally used for the treatment of inflammatory and rheumatic disorders. In the present study, density functional theory (DFT) calculations were employed to investigate the molecular geometry, electronic properties, and electrostatic characteristics of the phytochemical constituent heptadecane identified from the tuber extract. Geometry optimization was performed using the B3LYP functional with the 6-311++G(d,p) basis set, yielding energetically stable minimum-energy conformations with well-defined structural parameters. Frontier molecular orbital (HOMO-LUMO) analysis was carried out to evaluate the electronic behavior and reactivity trends of the compound. The calculated HOMO-LUMO energy gap indicates moderate electronic stability and limited chemical reactivity, consistent with the saturated hydrocarbon nature of heptadecane. Furthermore, molecular electrostatic potential (ESP) mapping was conducted to visualize the charge distribution over the molecular surface and to identify potential sites for electrophilic and nucleophilic interactions. The ESP analysis reveals a largely neutral electrostatic surface with minor charge variations along the carbon hydrogen framework, supporting the chemical stability of the molecule. Overall, the combined geometry optimization, frontier orbital, and ESP analyses provide meaningful molecular level insights into the stability and electronic features of *E. pursaetha* tuber-derived phytoconstituents.

*Keywords: DFT, orbital, E. pursaetha, chemical reactivity*

## 21. Innovation of Biodegradable Polymer from *Limonia Acidissima* Peel and Waste Newspaper Pulp

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### ABSTRACT

The increasing threat of plastic is a pressing issue, and increasing the use of biodegradable plastics is crucial. Decomposable plastics, made from *Limonia acidissima* peel, can significantly reduce the threat of non-degradable plastics. These decomposable plastics can be made using various materials, such as kotha powder, glycerine, gelatine, West newspaper, cornstarch, and polymer. Testing these films using various methods, such as FTIR, XRD, water absorption, and disintegration tests, can help determine their effectiveness.

*Keywords: Limonia acidissima, glycerine, gelatine*

## 22. Surface-Enhanced Raman Scattering Performance of Emerging Non-Noble and Hybrid Nanomaterials. A Study of Cu, Al, TiN, Graphene, and Perovskite Nanostructures

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### ABSTRACT

In this paper, the author is going to suggest a new hybrid mechanism of enhancing the Surface-Enhanced Raman Spectroscopy (SERS) activity by the using of both old and new materials of plasmonics and next-generation materials including copper (Cu), aluminum (Al), titanium nitrate (TiN), graphene oxide (GO) and perovskite nanocrystals. Such materials have been engineered to form hierarchical nanostructure to be in a position to exploit both the electromagnetic and chemical enhancement mechanisms to do so. Plasmonic interactions of local fields and affinity to insect implanted nanoparticles were amplified by plasmonic interactions during the formation of emerging semiconducting/ dielectric components and plasmonic metals by a large factor. The proposed substrates of SERS exhibited enhancement factors (EFs) of up to  $10^{-11}$  and a detection limit of the attomolar level. This type of implementation provides promising channels of multiplex sensing of biomedical diagnostics and environmental pollutant sensor which promises to the viability of alternatives to expensive and hyper sensitive Raman-based sensors.

*Keywords—Surface-Enhanced Raman Spectroscopy (SERS), Copper Nanostructures, Graphene Oxide, Titanium Nitrate, Perovskite Nanocrystals, Electromagnetic Enhancement, Chemical Enhancement, Hybrid Nanomaterials*

## 23. Modeling the Vagus Nerve as a Systemic Healing Regulator Using Graph Neural Networks

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### ABSTRACT

The vagus nerve plays a central role in regulating systemic inflammation, metabolism, and stress responses through distributed interactions between the brain and peripheral organs. Existing physiological models are largely reductionist and fail to capture the networked nature of vagal regulation. In this work, a graph neural network (GNN)-based theoretical framework is proposed to model the vagus nerve as a systemic healing regulator within a graph-structured physiological network. Organs and neural subsystems are represented as nodes, while vagal, hormonal, and inflammatory pathways form weighted edges. Healing is interpreted as a network-level dynamical and optimization process driven by vagal modulation. The proposed framework provides a mathematically grounded foundation for hypothesis generation, computational analysis, and the design of neuromodulation-based interventions.

*Keywords: vagus nerve, neural subsystems, mathematics*

## 24. Engineering pH-Responsive Graft Hydrogel Networks from Sterculia Gum for Functional Materials Applications

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### ABSTRACT

Stimuli-responsive hydrogels constitute an important class of soft functional materials whose performance is governed by the synergistic effects of network architecture, physicochemical interactions, and environmental conditions. In this study, a novel Sterculia gum/acrylamide/vinyl acetate hydrogel was synthesized via a graft copolymerization approach, integrating a renewable biopolymer backbone with synthetic polymer chains to achieve enhanced functional performance. The structural evolution and thermal behavior of the hydrogel were characterized using Fourier Transform Infrared (FTIR) spectroscopy and Differential Thermal Analysis (DTA), confirming successful grafting and improved network stability. The swelling behavior was systematically investigated as a function of time and pH (4.0, 7.0, and 9.2) at ambient temperature to establish structure–property relationships. The hydrogel exhibited pronounced pH-dependent swelling, attaining a maximum equilibrium swelling ratio of 12.63 g/g at pH 9.2, which is attributed to increased ionization and electrostatic repulsion within the polymer network. Swelling kinetics followed a non-Fickian diffusion mechanism, indicating that solvent transport and polymer chain relaxation occurred on comparable timescales which is a characteristic feature of viscoelastic polymer networks.

The combination of tunable swelling behavior, diffusion-controlled transport characteristics, and a biopolymer-based architecture makes this hydrogel a promising material for smart membranes, responsive coatings, controlled-release matrices, adsorptive systems for pollutant sequestration, and water-management technologies. Overall, this study provides valuable insights into the rational design of sustainable, pH-responsive hydrogel materials with tailored properties for advanced materials science applications.

**Keywords:** Stimuli-responsive hydrogels, Sterculia gum, Graft copolymerization, pH-dependent swelling, Non-Fickian diffusion, Structure–property relationship, Functional polymer networks.

*Keywords:* Biopolymer, hydrogels, non fickian diffusion

## 25. Synthesis of Aluminium Oxide Nanoparticles ( $\text{Al}_2\text{O}_3$ ) from Aluminium waste foils.

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### ABSTRACT

In this study, a new method is presented for synthesizing aluminium oxide nanoparticles ( $\text{Al}_2\text{O}_3$ ) from used aluminium foil, which contributes to the development of materials science and addresses waste management concerns. The process involves the treatment of aluminium foil with hydrochloric acid and sodium carbonate, leading to the production of  $\text{Al}_2\text{O}_3$  nanoparticles. Characterization of the nanoparticles was performed using UV-visible spectrophotometry, scanning electron microscopy (SEM), X-ray diffraction (XRD), and Fourier transform infrared spectroscopy (FTIR). The results revealed a yield of  $\text{Al}_2\text{O}_3$  nanoparticles at  $45.64 \pm 19.69\%$  with sizes ranging from 190-300 nm. UV-visible spectrophotometry demonstrated maximum absorption at 370 nm, while X-ray diffraction confirmed the crystalline structure. Characteristic vibration signals of  $\text{Al}_2\text{O}_3$  were identified through FTIR analysis. This method demonstrates an environmentally friendly way to repurpose aluminium waste for creating valuable nanomaterials, which could be utilized in diverse industries, aligning with the principles of a circular economy and sustainable waste management practices.

*Key Words: Aluminium Oxide Nanoparticles, Aluminium Foil, SEM, FTIR, XRD.*

## **26. Multifunctional Hausmannite (Mn<sub>3</sub>O<sub>4</sub>) Nanoparticles Synthesized via Hydrothermal Route for Antibacterial Applications**

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### **ABSTRACT**

Manganese oxide nanoparticles (Mn<sub>3</sub>O<sub>4</sub> NPs) have attracted significant attention due to their unique physicochemical properties and promising applications in biomedical and environmental fields. In the present study, Mn<sub>3</sub>O<sub>4</sub> nanoparticles were successfully synthesized via a facile hydrothermal method using manganese chloride tetrahydrate (MnCl<sub>2</sub>·4H<sub>2</sub>O) as a precursor. The hydrothermal approach offers advantages such as controlled particle size, high crystallinity, and simplicity of synthesis. The synthesized Mn<sub>3</sub>O<sub>4</sub> nanoparticles were comprehensively characterized using X-ray diffraction (XRD), ultraviolet–visible (UV–Vis) spectroscopy, Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and vibrating sample magnetometry (VSM). XRD analysis confirmed the formation of crystalline Mn<sub>3</sub>O<sub>4</sub> with a tetragonal spinel structure, indicating high phase purity. FTIR spectra exhibited a characteristic Mn–O stretching vibration, further validating the formation of manganese oxide. UV–Vis spectroscopy revealed a broad absorption band, attributed to electronic transitions within the Mn<sub>3</sub>O<sub>4</sub> nanoparticles. SEM images showed predominantly spherical nanoparticles with particle sizes ranging from 20 to 50 nm, while TEM analysis confirmed well-dispersed nanoparticles with an average size of approximately 30 nm. VSM studies demonstrated the magnetic behavior of the synthesized Mn<sub>3</sub>O<sub>4</sub> nanoparticles, suggesting their potential suitability for multifunctional applications. The antibacterial activity of the Mn<sub>3</sub>O<sub>4</sub> nanoparticles was evaluated against both Gram-negative *Escherichia coli* and Gram-positive *Staphylococcus aureus* using standard microbiological techniques. The results indicated significant antibacterial efficacy against both bacterial strains, which can be attributed to the nanoscale size, large surface area, and generation of reactive oxygen species by the Mn<sub>3</sub>O<sub>4</sub> nanoparticles. This study highlights the successful synthesis of Mn<sub>3</sub>O<sub>4</sub> nanoparticles with excellent structural, morphological, magnetic, and antibacterial properties, demonstrating their potential for biomedical and antimicrobial applications.

*Keywords : Hydrothermal, X-ray diffraction, Magnetic behaviour, Antibacterial activity and Biomedical applications*

## 27. *In-Vitro* Evaluation of *Cissus quadrangularis*, *Musa acuminata*, and *Phyllanthus emblica* Formulation for Microbial Inhibition and Wound Healing

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### ABSTRACT

Chronic wounds is different from acute wounds remain trapped in inflammatory phase result in production of excessive cytokines, proteases and reactive oxygen species, which impair tissue repair (Nagle et al., 2023). The polyherbal formulation was prepared incorporation with *Cissus quadrangularis*, *Phyllanthus emblica* and *Musa acuminata*. The preliminary phytochemical screening were evaluated the presence of rich bioactive substances. The sample were examined for alkaloids, flavanoids, sterols, terpenoids, anthraquinone, anthocyanin, proteins, phenolic compounds, quinones, carbohydrates, tannin, saponins, cardiac glycosides, glycosides, lignin, coumarins and volatile oils. The Hydro ethanolic formulation contains a significant number of phytochemical constituents, which contributes to antioxidant, anti-inflammatory and anticancer properties prevent the chronic diseases. Therefore, it has been selected further investigation. The polyherbal formulation characterization studies showed the presence of phenolic, flavonoids, aliphatic, aromatic, and carbonyl compounds as confirmed by UV-Vis, FTIR and GC-MS analysis attribute to strong antioxidant, antimicrobial and anti-inflammatory properties which enhance collagen synthesis, tissue regeneration and wound healing activity. The antioxidant activity of polyherbal formulation was determined by DPPH, NO and ABTS assays. The formulation shows the concentration dependent antioxidant activity. Therefore, the results strongly suggest that the polyherbal formulation made of three herbs displays the competent radical quenching effect which is much suitable for healing the wounds and tissue regeneration.

*Keywords* : Wounds, *Cissus quadrangularis*, *Musa acuminata*, and *Phyllanthus emblica*, Polyherbal

## 28. Optimization in the Era of AI: Techniques, Challenges, and Applications

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### ABSTRACT

Optimization techniques help solve complex problems in science, engineering, and machine learning by finding the best or nearly the best solutions. As data-driven and smart systems become more common, effective optimization is more important than ever. This paper reviews a range of optimization techniques, including classical methods, gradient-based approaches, heuristic and metaheuristic algorithms, and modern strategies used in machine learning. It looks at the strengths and weaknesses of each technique, where they are used, current challenges, and possible future research. This review aims to serve as a helpful resource for students, researchers, and practitioners.

### *Keywords*

*Optimization techniques · Gradient descent · Metaheuristic algorithms · Machine learning optimization · Swarm intelligence*

## 29. A Survey on Machine Learning–Based Feature Extraction Techniques for Image Processing and Computer Vision

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### ABSTRACT

Feature extraction plays a pivotal role in machine learning–driven image processing and computer vision systems. Raw image data are typically high-dimensional, noisy, and redundant, which makes direct learning inefficient and often ineffective. Feature extraction aims to transform raw pixel data into compact, discriminative, and task-relevant representations that improve learning accuracy, robustness, and computational efficiency. This survey provides an extensive review of machine learning–based feature extraction techniques with a primary focus on color, texture, and shape features. The paper systematically discusses the evolution from classical handcrafted descriptors to shallow machine learning–assisted representations and modern deep learning–based feature learning approaches. A detailed taxonomy, comparative analysis, and application-oriented discussion are presented, with special emphasis on domains such as medical imaging, remote sensing, and cyber-physical systems. Recent advances, challenges, and future research directions are also highlighted, making this survey a comprehensive reference for researchers and practitioners.

*Keywords -Feature extraction, machine learning, image processing, computer vision, color features, texture features, shape features, deep learning.2. Image Preprocessing for Texture Analysis*

### **30. Computationally Guided Design of Multifunctional Advanced Materials for Biomedical Applications**

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#### **ABSTRACT**

Biomedical implants and therapeutic devices are increasingly necessitating materials that can actively engage with biological systems while ensuring enduring mechanical and chemical stability. Problems like infections related to implants, poor tissue integration, inflammatory responses, and uncontrolled degradation still make it hard for doctors to be successful. Computationally guided materials design is a powerful way to deal with these problems and provide predictable biological performance. This paper examines the utilization of computational modeling tools in the design of advanced materials that incorporate biocompatibility, bioactivity, antimicrobial properties, and mechanical reliability. Multiscale modeling techniques, such as molecular dynamics simulations, density functional theory, and continuum-level analyses, are emphasized for their capacity to forecast protein adsorption, cell-material interactions, surface chemistry changes, and degradation behavior in physiological environments. These computational insights inform experimental approaches for enhancing material composition, surface topography, and functional coatings for use in orthopedic implants, cardiovascular devices, and tissue engineering scaffolds.

The computational design of multifunctional biomaterials that can inhibit bacterial colonization, promote osteointegration, and modify host immune responses is given particular attention. Large biological datasets are correlated with material properties using emerging machine learning and data-driven approaches, which allow for quick screening of potential biomaterials prior to in vitro and in vivo testing. Computational methods improve translational efficiency and regulatory readiness by lowering experimental uncertainty and speeding up material optimization. In general, a paradigm shift toward predictive, patient-focused biomaterial design is represented by the combination of computational modeling and biomedical materials science. This strategy encourages the creation of therapeutic materials and next-generation implants that are safer, more efficient, and suited to intricate biological settings.

#### *Keywords*

*Biomaterials; Biomedical implants; Computational modelling; Bio functional surfaces; Host– material interactions; Translational materials science*

## 31. Machine Learning and Multiphysics Modelling for Predictive Materials Design

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### ABSTRACT

Predictive design techniques that effectively capture multiscale structure–property–performance relationships are required due to the growing complexity of advanced material systems. By integrating data-driven intelligence with physics-based information, machine learning (ML) and multiphysics modeling have become a potent paradigm for accelerating materials discovery and optimization. For next-generation functional and multifunctional materials, this synergistic approach makes it possible to predict material behavior under coupled mechanical, thermal, chemical, electrical, and biological stimuli.

Recent developments in ML-assisted multiphysics modeling frameworks for predictive material design are examined in this paper. Property prediction, microstructure evolution, and process optimization are examined in relation to supervised and unsupervised learning algorithms, such as neural networks, random forests, Gaussian process regression, and deep learning architectures. In order to bridge length and time scales while maintaining physical consistency, these data-driven models are increasingly combined with phase-field modeling, density functional theory, molecular dynamics, and finite element methods.

Applications like smart biomaterials, energy storage systems, structural composites, and functional coatings, where multiphysics interactions dominate performance, are highlighted. Case studies show how ML-enabled surrogate models enable quick exploration of large design spaces by drastically lowering computational costs while preserving high predictive accuracy. Furthermore, hybrid modeling techniques and physics-informed machine learning are emphasized as cutting-edge methods for enhancing model interpretability, dependability, and extrapolation beyond accessible datasets.

A revolutionary change from trial-and-error experimentation to logical, data-driven materials engineering is represented by the combination of machine learning and multiphysics modeling. These methods are anticipated to be crucial in the creation of sustainable, high-performance materials for cutting-edge technological and biomedical applications by facilitating quicker optimization cycles, improved performance predictability, and well-informed decision-making.

### *Keywords*

*Machine learning; Multiphysics modeling; Predictive materials design; Data-driven materials science; Advanced materials*

## **32. Surface Roughness Analysis in Hard Turning of EN19 Steel Using Carbide Inserts with 0.4 mm Nose Radius**

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### **ABSTRACT**

This study presents an empirical investigation and optimization of surface roughness in the hard turning of EN19 alloy steel. Machining experiments were conducted on a rigid CNC lathe using CNMG carbide inserts with a fixed nose radius of 0.4 mm. Cutting speed, feed rate, and depth of cut were selected as the control parameters, while surface roughness was considered as the response variable. Response Surface Methodology (RSM) based on a Box–Behnken experimental design was employed to plan and analyze the experiments using Design-Expert® software. A total of 17 experimental runs were performed to develop an empirical model correlating machining parameters with surface roughness. Optimization was carried out using the desirability function approach to identify the optimal machining conditions. The results reveal that a minimum surface roughness value of 0.4081  $\mu\text{m}$  was achieved at a cutting speed of 1777.89 rpm, a feed rate of 0.0637 mm/rev, and a depth of cut of 0.147 mm. The developed model demonstrates good predictive capability and can be effectively applied to improve surface quality in the hard turning of EN19 steel.

*Keywords: Hard turning; EN19 alloy steel; Surface roughness; Carbide insert; Response surface methodology.*

### **33. Microbiological Assessment of Street Food: A Most Probable Number (MPN) Study on *Pani Puri* in Nashik**

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#### **ABSTRACT**

This project reports on the Microbial Assessment of Street Food: A Most Probable Number (MPN) Study on Pani Puri Sample. Pani Puri, a popular Indian street food, poses significant public health risks due to common poor hygiene and sanitation practices. The study's primary objective was to assess the microbiological quality of Pani Puri 'pani' (spicy water) collected from various street vendors. The Most Probable Number (MPN) method was employed to estimate the concentration of coliform bacteria, a critical indicator of fecal contamination. The methodology included the standard three phases: Presumptive Test, Confirmed Test (using Brilliant Green Lactose Bile broth ), and Completed Test (using Eosin Methylene Blue (EMB) agar ) to confirm the presence of fecal coliforms, specifically *E. coli*. The presumptive test results for four out of five samples showed a high MPN count of >900 per 100 ml , indicating microbial contamination. The Confirmed and Completed tests confirmed the presence of coliforms and growth on EMB plates, respectively. These findings highlight the significant public health risk associated with consuming such street foods, underscoring the urgent need for intervention to improve food safety practices among vendors, particularly concerning the use of unsafe water and poor personal hygiene.

*Keywords: Pani Puri, Street Food, Microbial Assessment, Most Probable Number (MPN), Coliforms, E. coli, Fecal Contamination, Public Health Risk*

### 34. Diversity and abundance of south Indian Spiders (Arachnida: Araneidae) collected from Villupuram, Tamil Nadu, India.

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#### ABSTRACT

The spider plays an important role in maintaining biological balance of nature. Stabilizing or regulating insect populations in recapture as well as in forest ecosystem. The present study was carried out for a period of six months from October 2024 to March 2025. The aim of study on Diversity of Araneidae spider's distribution from Villupuram District. In this study was understood that spiders are extremely abundant at natural habitat. In agro ecosystem they regulate the population of insect pests and other macro arthropods. They don't feed any part of the vegetation and do feed only the insects it. The study describes the identification of the spider assemblages with respect to their diversity and distribution in the agriculture area of Villupuram. A total of 10 species of spiders belonging to 7 genera under 5 families were recorded during the study period.

*Keywords: Spider, Diversity, Araneidae, Abundance, Macro arthropods.*

### **35. Lignin Peroxidase Mediated Green Synthesis of Silver Nanoparticle.**

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#### **ABSTRACT**

The synthesis of metallic nanoparticles (NPs) using eco-friendly green synthesis techniques is a promising alternative over chemical synthesis. The present study aims to develop sustainable and environment friendly approach for the synthesis of silver nanoparticle using extracellular lignin peroxidase enzyme from *Purpureocillium lilacinum* (LP8i). It has been proposed that a variety of proteins and enzymes are important for the creation of silver nanoparticles (Ag NPs) in fungi and bacteria. Partially purified lignin peroxidase from *Purpureocillium lilacinum* (LPi) released enzyme extract. The specific activity of the partly purified fraction is 126.61U/mg. XRD revealed face centered cubic (FCC) AgNPs with an average size of 84 nm after partially purified enzyme was exposed to silver nitrate solution. Synthesized Ag nanoparticles were characterized by UV-DRS, FTIR, FESEM- EDS, and XRD. This report describes the reduction of extracellular silver ions by fungal lignin peroxidase purified from *Purpureocillium lilacinum* (LPi).

*Keywords : by UV-DRS, FTIR, FESEM- EDS, and XRD*

## **36. Enhanced Supercapacitor Performance of Activated Carbon–Doped MXenes Synthesized Using Jackfruit Seed Biomass**

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### **ABSTRACT**

MXenes have gained significant attention as advanced electrode materials for supercapacitor applications due to their high electrical conductivity, layered morphology, and tunable surface chemistry. In the present work, MXenes doped with activated carbon derived from jackfruit seed biomass are synthesized and systematically investigated for electrochemical energy storage applications. The incorporation of biomass-derived activated carbon is intended to enhance surface area, porosity, and ion transport properties while promoting sustainable material utilization. The structural, morphological, and optical characteristics of the prepared MXene composites are examined using UV–Visible spectroscopy, Fourier Transform Infrared (FTIR) spectroscopy, X-ray Diffraction (XRD), and Scanning Electron Microscopy (SEM). The results confirm the successful formation of layered MXene structures with uniformly dispersed activated carbon, leading to improved interlayer spacing and enhanced electrolyte accessibility. Electrochemical performance is primarily evaluated using Cyclic Voltammetry (CV), Electrochemical Impedance Spectroscopy (EIS), and Galvanostatic Charge–Discharge (GCD) techniques. The CV analysis reveals a synergistic contribution of electric double-layer capacitance and pseudocapacitive behavior. EIS measurements demonstrate reduced charge-transfer resistance and improved ion diffusion kinetics, indicating efficient charge transport within the electrode material. GCD studies show high specific capacitance, good rate capability, and excellent cycling stability. The enhanced electrochemical performance is attributed to the synergistic interaction between MXenes and jackfruit seed–derived activated carbon, which provides abundant active sites and improved structural stability. This study highlights the potential of biomass-assisted MXene composites as efficient, sustainable electrode materials for next-generation supercapacitor applications.

*Keywords : MXenes; Activated carbon; Jackfruit seed biomass; Supercapacitor; Electrochemical energy storage*

### **37. Mechanistic Insights into NiO@rGO Nanohybrid-Induced Cytotoxicity via Oxidative Stress, Cell Cycle Arrest, and Apoptotic Pathways**

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#### **ABSTRACT**

NiO@rGO nanohybrids have gained significant interest across nanomedicine, energy storage, and environmental technologies due to the enhanced physicochemical performance achieved by integrating nickel oxide with reduced graphene oxide. Despite their expanding applications, concerns regarding their potential adverse effects on human health and the environment are increasing. While the toxicological profiles of individual nanoparticles such as NiO or rGO have been extensively investigated, comparatively little information is available on the biological impacts of their hybrid or composite counterparts. In this study, we evaluated the cytotoxic, oxidative stress-related, and apoptotic responses induced by hydrothermally synthesized NiO@rGO nanohybrids in normal rat kidney epithelial cells (NRK-52E). Structural and compositional analyses using XRD, TEM, and EDS confirmed the successful synthesis of high-purity nanohybrids with particle sizes ranging from approximately 24 to 28 nm, in which crystalline NiO nanoparticles were uniformly anchored onto rGO sheets. Cellular assays, including MTT, and morphological assessments, demonstrated a time- and concentration-dependent reduction in cell viability following NiO@rGO exposure. Furthermore, treated cells exhibited pronounced oxidative stress, characterized by elevated intracellular reactive oxygen species levels and depletion of glutathione. Evidence of apoptosis was observed through chromatin condensation, activation of caspase-3, formation of apoptotic bodies, and disruption of normal cell cycle progression. Collectively, these findings indicate that NiO@rGO nanohybrids elicit cytotoxic effects in mammalian cells primarily through oxidative stress-mediated apoptotic pathways.

*Keywords: Synthesis, Characterization, Cell viability, ROS, Caspase-3, Chromosome condensation, Cell death*

### 38. RN-I-OPEN SETS IN R-NEIGHBOURHOOD IDEAL SPACES

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#### ABSTRACT

In this paper, we introduce and study the concept of  $rn$ -I-open sets and define several new notions, namely  $rn$ -I-interior points and  $rn$ -I-cluster points, and investigate their fundamental properties. The relationships between  $rn$ -I-open sets and other existing classes of open sets are examined, and illustrative examples are provided to highlight the distinctions among these concepts. Further, we establish several characterizations and preservation properties of  $rn$ -I-open sets under set-theoretic operations. The majority of mathematical models play a crucial role in assisting society to resolve real-world problems, and general topology serves as an appropriate and flexible framework for modeling such problems. The results obtained in this paper contribute to the ongoing development of generalized topological spaces and open new directions for further research.

*Keywords :  $rn$ -I-open, general topology, flexible , framework*

### **39. Advanced Biomaterials: Bridging Biosciences for Functional and Regenerative Applications**

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#### **ABSTRACT**

In order to solve difficult problems in functional and regenerative applications, advanced biomaterials have evolved as a revolutionary class of materials that connects the biosciences, materials science, and biomedical engineering. Advanced biomaterials provide precise control over biological interactions at the tissue–material interface by combining concepts from cell biology, biochemistry, and molecular medicine with creative material design. These materials are designed to facilitate cell adhesion, proliferation, differentiation, and tissue remodeling by displaying specific physicochemical qualities, biocompatibility, bioactivity, and biodegradability. Bioactive ceramics, hydrogels, polymeric composites, smart and stimuli-responsive biomaterials, and nano-enabled systems that imitate the hierarchical structure and dynamic behavior of native extracellular matrices are examples of recent developments. These biomaterials are essential for wound healing, medication and gene delivery, tissue engineering, regenerative medicine, and implantable medical devices.

The functional adaptability of these materials has been further increased by the confluence of biosciences with modern fabrication techniques, such as surface functionalization, 3D bioprinting, and bio-inspired coating technologies. Furthermore, the creation of next-generation biomaterials that actively regulate biological responses and encourage long-term integration with host tissues is being guided by insights from stem cell biology, immunology, and mechanobiology. In addition to improving therapeutic results, this multidisciplinary approach speeds up the conversion of laboratory discoveries into solutions that are applicable to clinical settings. All things considered, sophisticated biomaterials serve as a vital link between the biosciences and regenerative technologies, providing individualized and sustainable methods for replacing, regenerating, and repairing damaged tissues and organs.

*Keywords: physicochemical qualities, biocompatibility, bioactivity, and biodegradability*

## 40. Biomass-Derived Activated Carbon from an Invasive Weed as a Functional Anode Material for Hydrogen-Based Electrochemical Cells

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### ABSTRACT

The growing demand for sustainable and low-cost electrode materials for hydrogen-based electrochemical energy systems has intensified research into biomass-derived carbons as alternatives to fossil-based carbon materials. In this work, activated carbon was synthesized from bio-char obtained from *Parthenium hysterophorus*, an aggressive invasive weed that poses severe ecological and agricultural challenges. The lignin-rich fraction of the biomass was converted into a carbonaceous precursor through integrated biomass fractionation, followed by controlled activation to enhance surface area, porosity, and surface functionality. The resulting activated bio-carbon exhibits a highly aromatic structure with micro- and mesoporous features, making it suitable for electrochemical applications requiring efficient charge transport and hydrogen interaction. Qualitative chemical tests and spectroscopic observations confirmed the formation of a stable carbon matrix with low inorganic residue, while the porous architecture is expected to facilitate hydrogen adsorption and electron transfer at the anode interface. Compared to conventional commercial carbon materials such as carbon black and synthetic activated carbons, the biomass-derived material offers significant advantages in terms of sustainability, feedstock availability, and cost-effectiveness. This study highlights the potential of invasive weed-derived activated carbon as a functional anode or anode-support material for hydrogen-based electrochemical cells. By converting an environmentally hazardous biomass into a value-added advanced material, the work demonstrates a sustainable waste-to-wealth approach that bridges biomass chemistry and hydrogen energy technologies. The findings provide a foundation for further electrochemical characterization and device-level evaluation of biomass-derived carbons in hydrogen energy systems.

*Keywords: Biomass-derived activated carbon; Parthenium hysterophorus; bio-charcoal; hydrogen energy; anode material; electrochemical cells; sustainable materials; invasive weed valorization*

## 41. Spider Silk: From Evolutionary Origins to Architectural Dynamics

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### **ABSTRACT**

The evolution of spider web construction is primarily determined by the balance between their behavioral patterns and material properties. This study is based on the analysis of various structures built by spiders, illustrating the interplay between self-produced materials such as silk and the environment. We present evidence supporting the hypothesis that self-produced materials exhibit greater uniformity and chemical complexity.

Combining biology and materials science, we observe that high-performance secreted polymers are essential for dynamic structures (such as prey-catching webs, filter net etc), while static structures (such as protective shelters) rely on the selection of environmental materials. This research also investigates the computational nature of construction behavior, where repetitive actions, combined with material constraints, give rise to complex structures.

During the research, it was observed that the Nephila web is highly advanced in nature, serving various purposes beyond hunting and providing inspiration for the design of advanced biomaterials.

*Keywords: spider Architecture; Bio-materials; Structural Evolution; Behavioral*

## 42. Potassium ion conducting nanocomposite polymer electrolytes: Synthesis, ion conduction and device fabrication

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### ABSTRACT

Preparation of a new K<sup>+</sup> ion conducting nanocomposite polymer electrolytes (NCPEs): (1-x) [70PEO:30KHCO<sub>3</sub>] + x SiO<sub>2</sub> where 0 ≤ x ≤ 30 wt.%, are reported. NCPEs were casted using a recently developed hot-press method. An order of conductivity jump was found in NCPEs by the complexation of nano-sized inert material SiO<sub>2</sub>. The material characterization was done with the help of Differential Scanning Calorimetric (DSC). Some important electrical properties viz. ionic conductivity ( $\sigma$ ), ionic mobility ( $\mu$ ), mobile ion concentration (n), ionic transference number ( $t_{ion}$ ) and activation energy have been characterized using different theories and models. A solid-state polymer cell is also prepared using the highest conducting composition of NCPE and cell performances were studied under various load conditions at different temperatures.

*Keywords: Nanocomposite polymer electrolyte; Ionic conductivity; DSC; Activation energy; Solid state polymer battery.*

### **43. *In Silico* and Nanoformulation Approaches to Curcumin-Mediated Glucansucrase Inhibition**

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#### **ABSTRACT**

Biofilm-mediated human infections present a significant healthcare concern in India, as traditional treatments are not working. A natural substance with therapeutic antibacterial qualities, curcumin has potential for use in clinical settings. The potential of curcumin as an inhibitor of *Streptococcus mutans*' extracellular polysaccharide (EPS) production—a crucial component in biofilm formation—is investigated in this work. The ligand (curcumin) and receptor (3AIC glucansucrase) structures were built using information from PubChem and RCSB-PDB, respectively, in order to evaluate this potential. Before molecular docking, the molecules were optimized and hydrogen atoms were added for accurate interaction analysis. Probe sonication was used to create curcumin nanoparticles. Sonication time, amplitude, initial macro-turmeric concentration, and solution pH were all optimized by repeated studies. Important discoveries showed that curcumin interacted with critical amino acids in the Active site of 3AIC glucansucrase. These interactions suggest that curcumin may be able to inhibit 3AIC glucansucrase. Curcumin's propensity to block the catalytic function of 3AIC Glucansucrase is further supported by the fact that 16 of the 19 necessary amino acids for the enzyme's catalytic activity showed similar interactions with curcumin. In summary, our study shows that curcumin can interact with important amino acids in 3AIC glucansucrase, thereby blocking its enzymatic activity and reducing the synthesis of EPS. Furthermore, curcumin nanoparticle manufacturing optimization provides important information for future research on its therapeutic effectiveness against infections linked to biofilms.

*Keywords: Molecular Docking, Nanocurcumin synthesis, Curcumin, Glucansucrase.*

#### 44. A Computational study of Non-linear optical crystal from bromoaniline

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#### ABSTRACT

Followed by one-pot mechanism Schiff base product derived from bromo aniline and crystallized by slow-evaporation technique. Crystal was characterized by Single crystal XRD analysis and it is in monoclinic system. The energy gap  $E_g$  was calculated by HOMO and LUMO and other theoretical parameters are determined using DFT method with B3LYP/6-311++ G (d,p) basis set. The supramolecular investigation of crystal structure explained by Hirshfeld analysis. Using quantum computations techniques, the topological parameters LOL and ELF, scatter graph and diagram of the crystal is the further characterization. The first order hyperpolarizability ( $\beta_0$ ) was calculated by B3LYP/6-311++ G (d,p) basis set. The first order hyperpolarizability value is greater than standard value of urea. Based upon this results crystal has outstanding nonlinear optical activity material and best for laser safety devices.

*Keywords: Crystal Explorer, ELF, DFT, NLO, Single crystal XRD*

## 45. A SPECTRAL GRAPH THEORETIC APPROACH TO CHEMICAL STABILITY

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### ABSTRACT

In these studies, the application of spectral graph theory helps in understanding chemical stability and aromaticity. Molecules are represented as graphs with atoms as vertices and bonds as edges. Spectral properties, such as eigenvalues and graph energy, are used to analyze molecular stability. Using examples like benzene and isobutane, the relationship between graph spectra and chemical behavior is explained. This work highlights the usefulness of graph theory as an effective tool in studying molecular structure and stability.

*Keywords: Spectral Graph Theory, Molecular Graphs, Chemical Stability, Aromaticity, Graph Theory, Adjacency Matrix, Eigenvalues, Graph Spectrum, Graph Energy,  $\pi$ -Electron Systems, Conjugation, Hückel Molecular Orbital (HMO) Theory, Molecular Connectivity, Electron Delocalization, Spectral Radius, Zero Eigenvalues, Molecular Stability, Chemical Reactivity, Benzene, Isobutane.*

## 46. A STATISTICAL STUDY ON TEA/COFFEE CONSUMPTION AND ITS IMPACT ON COGNITIVE PERFORMANCE AMONG G.T.N. ARTS COLLEGE STUDENTS

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### ABSTRACT

This study examines the pattern of tea and coffee consumption among college students and its impact on their cognitive performance. Data were collected from undergraduate students using a structured questionnaire, and statistical tools such as mean, median, standard deviation, correlation, t-test, and F-test were applied using Microsoft Excel. The analysis shows that moderate consumption of tea or coffee helps improve alertness and concentration, but excessive intake does not lead to better performance. The results also indicate that sleep hours and study habits have a stronger influence on cognitive performance than caffeine alone. The study highlights the importance of balanced caffeine intake along with healthy lifestyle habits for better academic performance.

*Keywords: Tea Consumption, Coffee Consumption, Caffeine, Cognitive Performance, College Students, Statistical Analysis, Mean, Standard Deviation, Correlation, t-Test, F-Test, Sleep Hours, Study Habits*

## 47. Inventory Optimization for Sustainable Advanced Material Supply Chains

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### ABSTRACT

The rapid adoption of advanced materials in modern manufacturing and biomedical industries has increased the complexity of inventory management due to high production costs, specialized storage requirements, and sustainability concerns. Traditional inventory models often fail to adequately capture the environmental and operational challenges associated with advanced material supply chains. This paper presents an inventory optimization framework for sustainable advanced material supply chains, integrating economic, environmental, and operational considerations. The proposed model incorporates sustainability-oriented factors such as carbon emissions, resource utilization, waste reduction, and material lifecycle characteristics alongside classical inventory costs. Advanced materials with unique physical and chemical properties are considered under demand uncertainty and limited storage conditions. Computational modelling techniques are employed to determine optimal inventory policies that balance cost efficiency with environmental performance. The results demonstrate that incorporating sustainability constraints into inventory decision-making leads to significant improvements in resource efficiency and emission reduction without compromising service levels. The proposed framework offers a practical decision-support tool for managing advanced material inventories and contributes to the development of sustainable and resilient material supply chains.

*Keywords: carbon emissions, resource utilization, waste reduction, material lifecycle*

## 48. Nickel (II), Copper (II), Cobalt (II) and Zinc (II) complexes of 4-hydroxy-3-methoxybenzaldehyde Semicarbazone: Synthesis, Characterization with Preliminary Anti-bacterial and Anti-fungal Activities

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### ABSTRACT

Semicarbazones have special chemical and biological characteristics that make them ideal for treating a variety of human illnesses. Vanillin semicarbazone complexes of Ni(II), Co(II), Cu(II), and Zn(II) are synthesized, and their spectral studies are provided. The metal forms coordinate bond with the azomethine nitrogen and covalent bond with the oxygen atom during process of metal complexation. A vanillin semicarbazone was synthesized by employing green approach taking water as solvent in the reaction of semicarbazide with appropriate carbonyl molecule. Metal complexes were synthesized by reacting corresponding metal chlorides with vanillin semicarbazone in 1:2 molar ratio. The newly synthesized complexes were examined, described, and compared to their parent ligands using  $^1\text{H-NMR}$ ,  $^{13}\text{C-NMR}$ , EDS, Mass spectroscopy and IR spectral methods. The anti-bacterial and antifungal screening conducted using derived complexes which demonstrated notable activity against all strains (*P. chrysogenum*, *F. oxysporum*, *E. coli* and *S. aureus*). The obtained outcomes specified that the produced complexes of metal may be attractive candidates for novel antibacterial and antifungal medicines, requiring additional biological investigations.

Keywords: *Synthesis, Semicarbazone, Metal complexes, Antibacterial activity, Antifungal activity.*

## 49. Advances in Coordination Chemistry with reference to Synthesis and Applications of Molybdenum and related Transition Metal Complexes from our Research Laboratory

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### ABSTRACT

Keeping in view the interesting structural variations and versatile applications of oxomolybdenum(VI) complexes, we have carried out some research work related to oxo- and dioxomolybdenum complexes in our research laboratory. Interaction of  $[\text{MoO}_2(\text{acac})_2]$  with internally functionalized oximes like  $\text{HON}=\text{C}(\text{CH}_3)\text{Ar}$  ( $\text{Ar} = \text{C}_4\text{H}_3\text{S}$ ,  $\text{C}_4\text{H}_3\text{O}$  or  $\text{C}_5\text{H}_4\text{N}$ ) and Schiff's Bases derived from  $\beta$  – diketones like  $\text{HOC}(\text{R})\text{CHC}(\text{R}')=\text{NC}_6\text{H}_5$  ( $\text{R} = \text{R}' = \text{CH}_3$  or  $\text{C}_6\text{H}_5$ ;  $\text{R} = \text{CH}_3$  and  $\text{R}' = \text{C}_6\text{H}_5$ ) in 1:2 molar ratio in  $\text{C}_2\text{H}_5\text{OH}$  has led to the formation of yellow dioxomolybdenum(VI) complexes of the type  $[\text{MoO}_2\{\text{ON}=\text{C}(\text{CH}_3)\text{Ar}\}_2]$  and  $[\text{MoO}_2\{\text{OC}(\text{R})\text{CHC}(\text{R}')=\text{NC}_6\text{H}_5\}_2]$ . Oximes were synthesized by green methodology. All newly synthesized products have been characterized by elemental analysis, IR, electronic,  $^1\text{H}$ ,  $^{13}\text{C}$  - NMR and FAB mass spectral studies.

Bioinformatics of a representative complex  $[\text{MoO}_2\{\text{ON}=\text{C}(\text{CH}_3)\text{C}_6\text{H}_4\text{N}\}_2]$  revealed that the molecule is likely to act on acetylcholine receptor and its anticandidal activity clearly reveals that complex is biologically active for fungal diseases.

On the other hand reactions of tetrachlorooxomolybdenum with sodium salts of internally functionalized oximes like  $\text{HON}=\text{C}(\text{CH}_3)\text{Ar}$  ( $\text{Ar} = \text{C}_4\text{H}_3\text{S}$ ,  $\text{C}_4\text{H}_3\text{O}$  or  $\text{C}_5\text{H}_4\text{N}$ ) and Schiff's Bases derived from  $\beta$  – diketones like  $\text{HOC}(\text{R})\text{CHC}(\text{R}')=\text{NC}_6\text{H}_5$  ( $\text{R} = \text{R}' = \text{CH}_3$  or  $\text{C}_6\text{H}_5$ ;  $\text{R} = \text{CH}_3$  and  $\text{R}' = \text{C}_6\text{H}_5$ ) in 1:2 molar ratio have been carried out in  $\text{CH}_3\text{CN}$ , which yielded dichlorooxomolybdenum (VI) complexes of the type  $[\text{MoOCl}_2\{\text{ON}=\text{C}(\text{CH}_3)\text{Ar}\}_2]$  and  $[\text{MoOCl}_2\{\text{OC}(\text{R})\text{CHC}(\text{R}')=\text{NC}_6\text{H}_5\}_2]$ . All newly synthesized products have been characterized by elemental analysis, IR, electronic,  $^1\text{H}$ ,  $^{13}\text{C}$  - NMR and FAB mass spectral studies.

Bioinformatics of two representative molecules  $[\text{MoOCl}_2\{\text{ON}=\text{C}(\text{CH}_3)\text{C}_5\text{H}_4\text{N}\}_2]$  and  $[\text{MoOCl}_2\{\text{OC}(\text{C}_6\text{H}_5)\text{CHC}(\text{C}_6\text{H}_5)=\text{NC}_6\text{H}_5\}_2]$  revealed that the molecules are likely to act on Serine Protease and Membrane Receptor sites, respectively. Further, pharmacokinetic properties of the molecules were also studied. In recent years similar type of complexes of the metals Cu(II), Ni(II), Zn(II) and Co(II) have also been synthesized in our research laboratory. Biological activities of newly synthesized metal complexes were carried out and results of initial investigations have been published in reputed SCI/ SCOPUS indexed journals. Such complexes may be constructed and organized to form crystals that contain large cavities. These porous materials are called metal–organic frameworks (MOF). By varying the building blocks used in the MOFs, these may be designed to capture and store specific substances. Nobel Prize of 2025 in Chemistry was awarded to Susumu Kitagawa, Richard Robson and Omar M. Yaghi for the development of metal–organic frameworks which can be used to harvest water from desert air, capture carbon dioxide, store toxic gases or catalyzed chemical reactions.

Keywords: *dioxomolybdenum (VI) complexes; Tetrachlorooxomolybdenum, Dichlorooxomolybdenum (VI) complexes, Internally functionalized oximes, Schiff's Bases derived from  $\beta$  – diketones, Pharmacokinetic properties, biological activities, metal–organic frameworks (MOF)*

## 50. Fuzzy Cognitive Map–Based Decision Making for Bio-Inspired Material Selection

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### ABSTRACT

Bio-inspired materials have emerged as promising candidates for advanced engineering and biomedical applications due to their adaptability, sustainability, and multifunctional properties derived from natural systems. Selecting an appropriate bio-inspired material involves complex decision making, as multiple interdependent criteria such as mechanical performance, biocompatibility, environmental sustainability, cost efficiency, and manufacturability must be considered simultaneously under uncertainty. This paper proposes a Fuzzy Cognitive Map (FCM)–based decision-making framework for the systematic selection of bio-inspired materials. The proposed approach models causal relationships among material attributes and performance objectives using fuzzy logic, enabling the representation of uncertainty, nonlinearity, and expert knowledge inherent in bioscience-driven material selection. Dynamic simulations of the FCM reveal the influence of key criteria on overall material suitability, allowing for transparent and interpretable decision support. The framework facilitates comparative evaluation of alternative bio-inspired materials and supports informed selection aligned with application-specific requirements.

The results demonstrate that FCM-based decision modelling offers an effective and explainable computational tool for bio-inspired material selection, bridging biosciences, advanced materials, and intelligent decision systems. The proposed methodology contributes to sustainable material design and supports interdisciplinary research in bio-inspired engineering and computational modelling.

*Key words: Bio-inspired materials, Fuzzy Cognitive Maps, Fuzzy logic, Multi-criteria decision making, Materia selection.*

## 51. Photocatalytic Degradation of Bromophenol Blue Dye and Antibacterial Activity of ZnO and Cu-Doped ZnO Nanoparticles

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### ABSTRACT

Green synthesis using plant extracts has emerged as a sustainable and cost-effective route for nanoparticle fabrication. In this work, ZnO and Cu-doped ZnO nanoparticles were synthesized via an eco-friendly co-precipitation method employing *Justicia adhatoda* leaf extract, achieving over 95% degradation efficiency toward a newly tested dye. X-ray diffraction analysis confirmed the formation of a hexagonal wurtzite ZnO structure with crystallite sizes of 21–22 nm. UV–Visible absorption studies revealed a reduction in the band gap from 3.1 eV for pure ZnO to 2.9 eV upon Cu doping, indicating enhanced optical absorption and photocatalytic performance. Fourier-transform infrared spectroscopy revealed that the functional groups in the leaf extract played a crucial role in nanoparticle formation. FE-SEM micrographs indicated a nanosheet-to-spherical morphology for ZnO, while Cu doping resulted in predominantly spherical particles. HR-TEM analysis, coupled with SAED patterns, confirmed the polycrystalline nature of the nanomaterials. X-ray photoelectron spectroscopy verified the presence of Zn<sup>2+</sup> and Cu<sup>2+</sup> oxidation states, demonstrating the successful incorporation of Cu into the ZnO lattice. The photocatalytic degradation efficiency of bromophenol blue is 96%, highlighting the noteworthy performance of this work. Furthermore, Cu-doped ZnO exhibited significantly enhanced antibacterial activity against *Bacillus subtilis* and *Staphylococcus aureus* compared to ZnO. Therefore, this green synthesis approach demonstrates strong potential for wastewater treatment and offers a sustainable strategy for future household wastewater management.

Key words: Zinc; Copper; Photocatalysis; Dye degradation; *Justicia Adhatoda*; Bromophenol Blue dye; *Bacillus subtilis*;

## 52. High-Efficient Gate Diffusion Input-Based Approximate Full Adders with Image Processing Application

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### ABSTRACT

This research details the development of ultra-compact approximate Full Adders (FAs) designed to optimize hardware efficiency through the strategic sacrifice of computational precision. By integrating Gate Diffusion Input (GDI) logic with Carbon Nanotube Field-Effect Transistors (CNTFETs) and Dynamic Threshold (DT) techniques, these designs effectively mitigate the threshold voltage drop common in low-transistor circuits. Three novel approximate FAs are proposed, featuring transistor counts of 8, 4, and 2, and named Cell-1, Cell-2, and Cell-3, respectively. All three circuits exhibit four errors, but their error distribution is distinctive, and they utilize different gate-level structures compared to references. The gate diffusion input (GDI) gates varying mean relative error distances (MREDs). Cell-1 has an MRED of 0.3541, while Cell-2 and Cell-3 achieve a value of 0.3125. These circuits demonstrate notable performance by the GDI, dynamic threshold (DT), and the incorporation of carbon nanotube field-effect transistors (CNTFETs) to address threshold voltage drop challenges. Regarding power-delay product (PDP), the best circuits are Cell-2 and Cell-3. A 35.41% improvement is seen by Cell-3 compared to Cell-2 and a 6.89% lower energy gained by Cell-2 compared to the nearest competitor. Cell-2 demonstrates the best performance when embedded in the proposed multiplier. In practical applications of image addition and finite impulse response (FIR) filtering of an electrocardiogram (ECG), the FAs make efficient 10-bit ripple carry adders (RCAs).

*Keywords* Approximate computing · Full adder · Gate diffusion input · Multiplier · FIR filter

## **53. Biodegradable Electronics and Eco-Materials: A Sustainable Pathway for Future Electronic Technologies**

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### **ABSTRACT**

The exponential growth of electronic devices has intensified the global challenge of electronic waste, creating serious environmental and health concerns due to the widespread use of non-renewable and non-degradable materials in conventional electronics. In this context, biodegradable electronics and eco-materials have emerged as a sustainable alternative, offering the possibility of functional electronic systems that safely decompose after their intended lifespan. This paper provides a comprehensive review of recent advances in biodegradable electronics, focusing on environmentally benign materials, fabrication techniques, functional performance, and application domains. The study examines a wide range of eco-materials, including biodegradable polymers, natural substrates, organic semiconductors, and transient conductive materials, highlighting their roles in the development of sustainable electronic components. Fabrication strategies such as solution-based processing and printing technologies are discussed with respect to their environmental advantages and scalability. Key application areas, including implantable biomedical devices, environmental monitoring systems, and disposable consumer electronics, are analysed to illustrate the practical relevance of biodegradable electronic technologies. Furthermore, the paper addresses critical challenges related to material stability, electrical performance, controlled degradation, and large-scale manufacturing. Future research directions are explored, emphasizing the integration of biodegradable electronics into circular economy frameworks and green manufacturing practices. Overall, this study underscores the potential of biodegradable electronics and eco-materials to significantly reduce electronic waste, promote responsible innovation, and support the transition toward sustainable and environmentally conscious electronic technologies.

*Keywords: Biodegradable Electronics, Eco-materials, Sustainable Electronics, Green Technology, Electronic Waste, Transient Devices*

## 54. Bridging the Realms of Mathematics and Chemistry: A Comprehensive Theoretical and Applied Study of Degree-Based Topological Indices

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### ABSTRACT

Degree-based topological indices are important tools in mathematical chemistry for measuring molecular structure and predicting physicochemical properties. This study offers a detailed comparison of three key degree-based indices: the first and second Zagreb indices ( $M_1$  &  $M_2$ ), the Randic index ( $R$ ), and the Harmonic index ( $H$ ), across various types of graphs. Through careful mathematical work and computational testing, we establish clear expressions and relationships among these indices for path, cycle, complete, and regular graphs. The results show that for all regular graphs,  $R(G)$  equals  $H(G)$ , which suggests a structural overlap in highly symmetric molecular systems. On the other hand, for trees and irregular graphs, different behavioural patterns appear, with the Harmonic index often displaying stronger links to physical properties like boiling points and molecular strain energy. Additionally, we present new bounds and inequalities that define the relative sizes of these indices, offering greater insight into their structural sensitivity. These findings lay a theoretical foundation for effectively choosing and using degree-based descriptors in QSPR/QSAR modelling, enhancing predictive reliability and limiting redundancy in chemical graph theory.

*Keywords: Degree-Based Indices, Zagreb Indices, Randic Index, Harmonic Index, Topological Descriptors, Chemical Graph Theory, QSPR/QSAR, Regular Graphs, Molecular Structure, Structure–Property Relationships*

## 55. $\text{Ca}_2\text{V}_2\text{O}_7/\text{ZnO}$ nanocomposite: A Novel Electrode for Battery & Supercapacitor applications

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### ABSTRACT

The design and engineering of multifunctional nanomaterials for advanced energy-related applications are of growing importance. In this context, a novel calcium vanadate–zinc oxide ( $\text{Ca}_2\text{V}_2\text{O}_7/\text{ZnO}$ ) nanocomposite was successfully synthesized using a straightforward solution combustion method. X-ray diffraction (XRD) analysis confirmed the formation of triclinic  $\text{Ca}_2\text{V}_2\text{O}_7$  and hexagonal ZnO phases, further supported by density functional theory (DFT) data from the Materials Project. Ultraviolet diffuse reflectance spectroscopy (UV-DRS) indicated a major electronic transition corresponding to a reduced bandgap energy of 2.4 eV. X-ray photoelectron spectroscopy (XPS) analysis validated the elemental composition and possible interactions among the composite's constituents.

A modified carbon paste electrode incorporating the  $\text{Ca}_2\text{V}_2\text{O}_7/\text{ZnO}$  nanocomposite was fabricated to investigate its electrochemical performance. The electrode's behavior was characterized using cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS), demonstrating a high specific capacitance of 1024 F/g at a current density of 2 A/g. These findings highlight the  $\text{Ca}_2\text{V}_2\text{O}_7/\text{ZnO}$  nanocomposite's excellent energy storage capabilities and its potential application in next-generation supercapacitor devices.

*Keywords:  $\text{Ca}_2\text{V}_2\text{O}_7/\text{ZnO}$  nanocomposite, Supercapacitor*

## 56. Comparative Analysis of Naive Bayes and Support Vector Machine Algorithms for Diabetes Prediction

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### ABSTRACT

Diabetes mellitus is a pervasive metabolic disorder with substantial morbidity and mortality worldwide. Accurate and early prediction is critical for effective clinical intervention. This study presents a comparative evaluation of two supervised machine learning algorithms—Naive Bayes (NB) and Support Vector Machine (SVM)—for predicting diabetes using the Pima Indian Diabetes dataset. Models were assessed via different parameters including accuracy, precision, recall, F1-score, and ROC-AUC metrics. Experimental results which demonstrate that SVM outperforms the NB in predictive accuracy, whereas NB offers computational efficiency and interpretability. The study highlights the trade-offs between model complexity and performance, providing actionable insights for selecting suitable predictive models in healthcare applications. These findings contribute to the development of robust, data-driven decision support systems for early diabetes diagnosis.

*Keywords-* Diabetes Prediction, Machine Learning, Naive Bayes, Support Vector Machine, Classification, Healthcare Analytics, Predictive Modeling, Medical Data Mining

## 57. COMPUTATIONAL VERIFICATION OF TORRICELLI'S LAW: INTEGRATING PYTHON ANALYSIS WITH FLUID DYNAMICS

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### ABSTRACT

Torricelli's law explains the velocity of liquid flowing through a small orifice at the bottom of a container, stating that the efflux velocity is proportional to the square root of the liquid height above the orifice, as derived from Bernoulli's principle under ideal flow conditions. This paper computationally verifies Torricelli's law using Python to model fluid flow, analyze the relationship between height and velocity and simulate discharge behavior. Theoretical equations are implemented using NumPy and Matplotlib and the computational results show close agreement with theory, with minor deviations due to real-world effects such as viscosity, friction, and energy losses.

*KEYWORDS : Torricelli's Law, Fluid Dynamics, Bernoulli's Principle, Python Programming, NumPyMatplotlib, Computational Modeling, Numerical Simulation*

## 58. Geodetic Domination on Consecutive clique of Size-3

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### ABSTRACT

In this Paper we study the geodetic and geodetic domination number of consecutive cycles of size-3. The geodetic set and Geodetic dominating set of these graphs are obtained. We also studied and proved the results on minimum geodetic number and minimum geodetic domination number of these graphs. Also, the results obtained are illustrated by graphs.

*Keywords: geodetic number, size-3, geodetic domination*

## 59. In Silico Investigation of 5-Substituted 1H-Tetrazole Derivatives: Molecular Docking and PASS Analysis

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### ABSTRACT

As considering importance of 5-substituted 1H-tetrazole derivatives which is class of nitrogen rich heterocyclic compounds for their biological and pharmaceutical applications. In the present study we focused to investigate the in silico biological activities of selected 5-substituted 1H-tetrazole derivatives obtained using hydrothermally synthesised Cu-doped indium Oxide as an efficient heterogeneous catalyst. The catalyst was synthesised using hydrothermal method and characterised using various tools and found excellent morphology with orthorhombic having particle size 16.31 nm (matches with JCPDS card No. - 73-1592), while the BET analysis proves the surface area 183720 cm<sup>2</sup> g<sup>-1</sup>. The main objective of this work is to evaluate the interaction of synthesised derivatives with selected biological targets and to predict their pharmacological activities through computational approach. Molecular docking studies were performed by the use of CB Dock-2 to find the binding affinity and interaction of ligand with targeted proteins of antioxidant enzyme, anti-inflammatory enzyme, and anti-cancer protein. In addition to this prediction of activity spectra for substances (PASS) was studied to find possible biological activities and toxicity of synthesised derivatives which is based on their structural features. The combined molecular docking and PASS analysis supports their candidacy for further *in vitro* and *in vivo* biological evaluation, highlighting the significance of Cu-doped indium oxide-assisted synthesis in developing biologically relevant heterocyclic compounds.

*Keywords: Hydrothermal Synthesis; Heterogeneous catalysis; Tetrazole; Molecular Docking; PASS.*

## 60. GRAPH THEORETICAL MODELING AND ANALYSIS OF ELECTRIC CIRCUIT USING MATLAB

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### ABSTRACT

In this paper, a graph theoretical approach is used to model and analyze electric circuits in a simple and systematic way. In graph theory, the electric circuit is represented using nodes (vertices) and branches (edges), which makes the analysis easier and more organized. The given electric circuit is first converted into a graph model. From this graph, important matrices such as the incidence matrix, tie-set matrix, and cut-set matrix are formed. These matrices help in applying Kirchhoff's Current Law (KCL) and Kirchhoff's Voltage Law (KVL) to analyze the circuit. The entire modelling and analysis process is implemented using MATLAB, which helps in performing calculations quickly and accurately. MATLAB simulations are used to find branch currents and node voltages of the electric circuit. The results obtained using graph theory are compared with conventional methods to verify correctness.

### *Keywords*

*Electric circuits ,Nodes, Branches ,Kirchhoff's Current Law, Kirchhoff's Voltage Law Graph Theory, Adjacency Matrix, Eigenvalues, IncidenceMatrix , LaplacianMatrix ,MATLAB ,Conductance*

## 61. GRAPH THEORY AND ITS APPLICATION IN PROTEIN–PROTEIN INTERACTION NETWORKS

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### ABSTRACT

Graph theory provides a powerful mathematical framework for analyzing complex biological systems. In this paper, protein–protein interaction (PPI) networks are modeled using graph-theoretical concepts, where proteins are represented as vertices and their interactions as edges. The study focuses on analyzing important network properties such as degree distribution, connectivity, clustering coefficient, and centrality measures to identify key proteins within the network. Graph-based analysis helps in understanding the structural organization and functional behavior of biological systems. This approach is useful in identifying hub proteins, understanding disease mechanisms, and supporting drug target discovery. The paper highlights the significance of graph theory as an effective analytical tool in bioinformatics and systems biology.

*Keywords: Graph Theory, Protein–Protein Interaction, Biological Networks, Network Analysis, Bioinformatics*

## **62. Preparation and Characterization of Transparent NiO and Cobalt Doped NiO Thin films by Spray Pyrolysis Technique**

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### **ABSTRACT**

Transparent Nickel oxide (NiO) and Cobalt (Co) doped nickel oxide thin films with oriented growth along (111) plane were deposited onto glass substrates at the temperature of 350° C by spray pyrolysis technique using moisture filtered air as carrier gas. The effect of cobalt doping on structural, optical and morphological properties were analysed. The crystallinity and structural characteristics of the pure and cobalt doped NiO thin films were carried out through X-ray diffraction (XRD). Oxidation states and chemical compositions of NiO and Co doped NiO thin films were analysed by calculating the binding energy from X-ray Photoelectron spectroscopy (XPS). Optical properties of the prepared films were analysed through UV-Vis transmittance spectra. The films have good transparency in the visible and near infra-red region. Band gap values were estimated by plotting the absorption coefficient versus incident photon energy curves. Non-linear absorptive studies were performed through Z-scan technique. Morphological analysis was carried out through Field emission scanning electron microscopy (FESEM). The elemental composition and the presence of Co dopant in the prepared films were confirmed from Energy Dispersive X-ray spectroscopy (EDS) results.

*Key words: Nickel oxide thin films; Spray pyrolysis method; oriented growth; transparent films; cobalt doping*

### **63. Web-Based Classification System for Automated Identification of Martian Surface Features from HiRISE Imagery**

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#### **ABSTRACT**

The automated Mars orbital interpretation of images is vital towards enhancing the study of the surface of the planet. This study introduces a viable implementation system of categorizing the surface features of Mars using the images of the HiRISE into a convenient web-based platform. After extensive testing of various deep learning models to detect seven categories of surface features, namely, craters, bright and dark dunes, slope streaks, impact ejecta, swiss cheese and spider formations, the selected model was an optimized classification model. The system has an easy-to-use interface that allows researchers and planetary scientists to post HiRISE images and receive automatic classification in real-time. To make dependable classification, the implemented model will have uncertainty-detecting mechanisms that identify unclear classifications enabling users to make wise decisions concerning the validity of results. It is a web-based system that democratizes advanced Mars surface classification techniques and does not require specialized machine learning knowledge or computational infrastructure. The system can be utilized in the continuation of the exploration of the planet by filling the gap between theoretical knowledge and application in practice, thus providing quick analysis of orbital data of Mars. This system demonstrates the viability of translating research-grade deep learning models into accessible tools for the planetary science community, paving the way for collaborative, large-scale analysis of Martian orbital datasets.

*Keywords: Deep Learning, HiRISE, Web-based system.*

## **64. Multiscale Computational Modeling of Coupled Physical, Chemical, and Biological Systems**

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### **ABSTRACT**

Computational modeling has emerged as a unifying methodology for addressing complex scientific problems that span multiple disciplines. This work explores computational methods for cross-domain modeling in the physical and biological sciences, with an emphasis on integrating principles from physics, chemistry, and biology within a unified computational framework. Physical systems are governed by fundamental laws such as classical and continuum mechanics, thermodynamics, and electromagnetism, whereas biological systems are characterized by biochemical interactions, regulatory networks, stochastic processes, and multiscale organization. Bridging these domains requires advanced computational techniques capable of handling heterogeneous data, nonlinear interactions, and multiple spatial and temporal scales.

*Keywords: Index Terms—Multiscale modeling, computational modeling, physical systems, chemical kinetics, biological systems, coupled systems.*

## 65. Optimization in the Era of AI: Techniques, Challenges, and Applications

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### ABSTRACT

Optimization techniques help solve complex problems in science, engineering, and machine learning by finding the best or nearly the best solutions. As data-driven and smart systems become more common, effective optimization is more important than ever. This paper reviews a range of optimization techniques, including classical methods, gradient-based approaches, heuristic and metaheuristic algorithms, and modern strategies used in machine learning. It looks at the strengths and weaknesses of each technique, where they are used, current challenges, and possible future research. This review aims to serve as a helpful resource for students, researchers, and practitioners.

*Keywords: Optimization techniques · Gradient descent · Metaheuristic algorithms · Machine learning optimization · Swarm intelligence*

## 66. Modeling Treatment of Cancer using Oncolytic Virotherapy with T-Helper cells

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### ABSTRACT

In this paper, we introduce a simple mathematical model by logistic growth of tumor cells and simple mass-action type incidence between virus and uninfected tumor cells. Additionally, we incorporate latent delay in conversion of uninfected tumor cells to virus infected tumor cells. Hence in this paper we formulate a mathematical model for the treatment of cancer by incorporating two delays, namely, latent delay and delay in activation of CTLs due to T-helper cells. This model seems to be more realistic though there is scope to further improve it by considering saturation type incidence and generalized logistic growth of tumor cells. Here we aim to see the impact of delay on treatment of cancer using virotherapy. Here we also explore the case when one of the delay is zero. The proposed model looks simple but it exhibits complex dynamics due to the presence of delay. Numerical simulation is performed to support the analytical findings.

*Keywords : Cancer, Virotherapy, Hopf-Bifurcation*

## 67. MILDLY $R$ -NEIGHBOURHOOD $I_g$ -CLOSED SETS

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### ABSTRACT

In this paper, we introduce and study the concepts of mildly  $r$ -neighbourhood  $I_g$ -closed sets, weakly  $r$ -neighbourhood  $I_g$ -closed sets, strongly  $r$ -neighbourhood  $I_g$ -closed sets,  $r$ -neighbourhood ideal topological spaces and investigate some of its basic properties and characterization.

*Keywords : closed sets,  $r$ -neighbourhood*

## 68. Seeing Through Sound: Smart Goggles for Visually Impaired Kids

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### ABSTRACT

This research presents a smart wearable goggle system designed to assist visually impaired children by improving environmental awareness, safety, and supervised independence. The proposed system integrates a camera, Raspberry Pi processor, GPS–GSM module, rechargeable battery, and audio output into a lightweight goggle form factor suitable for children. Real-time object detection is performed using a YOLOv8 deep learning model trained on India-specific hazards such as potholes, stray animals, and auto-rickshaws. In addition to object recognition, the system incorporates facial recognition to identify pre-registered trusted individuals and log interactions with unknown persons. A GPS-based geofencing mechanism allows parents or guardians to define safe zones and receive alerts if boundaries are crossed. Additional safety features include live location tracking, height-based differentiation between adults and children, emergency SOS alerts, impact-based damage detection, and intelligent battery monitoring. All processing is optimized for offline operation, ensuring low latency, data privacy, and reliability in environments with limited internet connectivity. The proposed system addresses key limitations of existing assistive technologies by combining localized AI perception, personalization, and parental monitoring into a single child-centric wearable solution.

*Keywords: Smart Goggles; Visually Impaired Children; YOLOv8; Object Detection; Facial Recognition; Geofencing; Voice Feedback*

**69. STATISTICAL ANALYSIS OF TUBERCULOSIS CASES IN SHANARPATTI  
BLOCK (2022–2024)**

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**ABSTRACT**

In this study, tuberculosis (TB) data were collected from the Primary Health Centre (PHC), Shanarpatti Block. Statistical tools were applied using Python programming to analyse the data and to construct statistical problems through hypothesis testing. The study also aims to create awareness among young minds about tuberculosis prevention and control. As part of social responsibility, the findings along with suitable suggestions were submitted to the Block Health Office (BHO).

*Keywords: Tuberculosis, Statistical Analysis, Shanarpatti Block, Primary Health Centre Data, Descriptive Statistics, Inferential Statistics, Z-Test, F-Test, Python Programming, Public Health.*

## **70. UNDERSTANDING THE USER EXPERIENCE IN ONLINE FOOD DELIVERY APPLICATION**

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### **ABSTRACT**

Food delivery applications have revolutionized the way people access and consume food in the modern era. The convenience and accessibility offered by these platforms have significantly influenced eating habits, lifestyle patterns, and spending behaviors. The frequent use of food delivery apps may impact individuals' health, time management, and financial stability. The growing dependency on such platforms has become a notable trend among college students. This study investigates the usage of food delivery applications among GTN College students, exploring attitudes and practices related to food delivery services. A questionnaire was created using Google Forms. This study contributes to the existing body of research on food delivery applications among young adults. Using ANOVA, this study investigated the demerits of several platforms among GTN Arts College students, identifying significant variations in attitude and behaviors towards food delivery applications.

*KEYWORDS: Consumer behavior, pricing transparency, discounts, loyalty systems, Sample mean, Population mean, sample standard deviation, population standard deviation, critical region, null hypothesis and alternative hypothesis.*

## 71. INNOVATIVE SHAPE MEMORY MATERIALS FOR TECHNICAL APPLICATIONS

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### ABSTRACT

Shape memory materials are defined as a “family of materials that can change their shape from deformed shape to their programmed original shapes”. The recovery in shape is achieved by the surrounding temperature and various other stimuli like: ultraviolet light, electric field, pH, magnetic field or by specific chemicals. The research review deals with the implementation of innovative materials in developing shape memory mechanism for various technical applications. Materials used in developing shape memory materials can be organic and inorganic based on their composition and constituents. Inorganic materials contain ceramics and alloys. Organic material contains gels and polymers. For biomedical applications, nickel titanium (nitinol) is identified as a successful material for shape memory mechanism. It is widely used in stent for heart patient and orthodontic wires for dental use. Staples and clamps made of nitinol used for fastened the fracture bones inside the human body. In clothing and textile field, specific brassiere is made of shape memory materials which give good comfort, look and serviceability property. Shape memory wires or springs were incorporated in sleeves, handbags, suitcases to enhance the aesthetic appearance. It is reported that around 30 % of protection increases when shape memory material is implemented in fireproof jackets. In aerospace applications, shape memory material successfully used in the cryofit hydraulic couplings which is commercialized as a “aerofit”. Shape memory material is widely in the micro robotic systems specifically for the joint design and artificial muscle design. In sportswear, specific sensors are connected to the shape memory material that can provide functional properties like improvement in fitness, temperature and creating the adaptive environment. Shape memory fibers are used in the compression garments during post operative condition and healing of injured tissues. It can be concluded from the study shape memory fibers, polymers, alloys open new opportunities for developing smart, transformable and functional materials. Moving towards sustainability, it is suggested that more ecofriendly novel agrowaste fibers can also be used in shape memory materials.

*Keywords : Shape, Memory, Technical, Material*

## **72. Computational Analysis and Molecular Docking of Bioactive Compounds from *Strobilanthes glutinosus* Targeting the HER2 Receptor**

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### **ABSTRACT**

*Strobilanthes glutinosus* is a medicinal plant with limited scientific exploration despite its traditional therapeutic relevance. The present study aims to investigate the anticancer potential of bioactive compounds derived from *Strobilanthes glutinosus* through computational analysis and molecular docking against the Human Epidermal Growth Factor Receptor-2 (HER2), a well-established therapeutic target in breast cancer. Phytochemical constituents reported from *Strobilanthes glutinosus* were screened for drug-likeness using Lipinski's Rule of Five and ADMET prediction tools to evaluate their pharmacokinetic and toxicity profiles. The selected compounds were subjected to molecular docking studies against the HER2 receptor to assess binding affinity and interaction patterns. Docking results revealed that several bioactive compounds exhibited strong binding energies and stable interactions with key amino acid residues at the active site of the HER2 receptor, comparable to standard inhibitors. These findings suggest that *Strobilanthes glutinosus* harbors promising lead compounds with potential HER2 inhibitory activity. The study provides a computational foundation for further in vitro and in vivo validation of these phytochemicals as prospective anticancer agents targeting HER2-positive breast cancer.

**Keywords:** *Strobilanthes glutinosus*, Lipinski's Rule, ADMET prediction, Molecular Docking

### 73. Green synthesis of silver nanoparticles with potent anticancer activity using

#### *Phyllanthus emblica* leaf extract

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#### ABSTRACT

Silver nanoparticles (AgNPs) have emerged as promising materials because of their unique physicochemical characteristics and their increasing importance in biomedical applications. However, traditional chemical methods for nanoparticle synthesis often involve toxic reagents that pose risks to both the environment and human health. This has led to a growing interest in environmentally sustainable and safer green synthesis strategies. In this study, *Phyllanthus emblica* leaf extract, which is naturally enriched with phenolic and flavonoid compounds and exhibits strong anticancer activity ( $IC_{50} \approx 80 \mu\text{g mL}^{-1}$ ), was employed as a natural reducing and stabilizing agent for the fabrication of AgNPs. The successful synthesis was visually evident from the rapid transformation of the  $\text{AgNO}_3$  solution color from light to dark brown after the addition of the plant extract. The biosynthesized *P. emblica*-AgNPs were characterized by UV-visible spectroscopy, displaying a characteristic absorption peak at 403 nm, Zeta potential analysis showing high stability with a value of  $-48.3$  mV, and HR-SEM analysis, which indicated an average particle size of approximately 31 nm. The synthesized nanoparticles exhibited significant antiproliferative activity against lung cancer (A-549) cells, achieving about 42% inhibition of cell growth even at lower concentrations. Furthermore, fluorescence microscopic examination using PI staining revealed marked nuclear and cellular morphological changes in treated cells, confirming anticancer potential of the green-synthesized AgNPs.

**Key Words:** Green synthesis, *Phyllanthus emblica*, AgNPs, Anticancer activity, A-549 Cell

## 74. RECENT ADVANCES IN THE SYNTHESIS AND APPLICATIONS OF CONDENSED Beta-Lactam

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### ABSTRACT

Condensed Beta-Lactam have gained significant attention in recent years due to their broad-spectrum antimicrobial activity, resistance to  $\beta$ -lactamases, and versatility as synthetic intermediates. Since 2000, extensive research has focused on developing efficient methodologies for their synthesis, primarily through cyclization reactions of functionalized monocyclic  $\beta$ -lactams using metal salts or halocyclization techniques. These compounds play a crucial role in the development of novel antibiotics and functionalized heterocycles, making them valuable in both pharmaceutical and synthetic chemistry.

This review provides an overview of nonconventional condensed  $\beta$ -lactams, highlighting key synthetic strategies and their advantages under different conditions. With the rising demand for new antimicrobial agents, condensed Beta-Lactam hold promise for addressing antibiotic resistance and expanding the arsenal Beta-Lactam-based drugs. This work aims to guide researchers by summarizing recent advancements, exploring emerging trends, and discussing future perspectives in condensed Beta-Lactam synthesis and applications.

**Keywords-** antibiotics, azetidinones, penicillin, cephalosporin, peptidases

## 75. A Data-Driven AI Approach for Liver Cancer Prediction and Survival Analysis

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### ABSTRACT

Liver cancer remains one of the leading causes of cancer-related mortality worldwide, primarily due to late diagnosis and limited personalized prognostic strategies. This study presents a data-driven artificial intelligence (AI) approach for liver cancer prediction and survival analysis by integrating clinical, imaging, and pathological data. Advanced machine learning and deep learning models are employed to accurately identify liver cancer patterns and predict patient outcomes. Convolutional Neural Networks (CNNs) are utilized for automated feature extraction from medical imaging data, while statistical and machine learning based survival models, including Cox Proportional Hazards and deep survival networks, are applied to estimate patient survival probabilities. The proposed framework emphasizes data pre-processing, feature selection, class imbalance handling, and model optimization to improve predictive robustness and generalizability. Performance evaluation is conducted using standard metrics such as accuracy, precision, recall, F1-score, area under the ROC curve (AUC), and concordance index for survival prediction. Experimental results demonstrate that the data-driven AI models outperform traditional statistical approaches in both liver cancer detection and survival outcome prediction. Moreover, explainable AI techniques are incorporated to enhance model transparency and support clinical interpretability. This research highlights the potential of AI-assisted decision support systems to aid clinicians in early diagnosis, risk stratification, and personalized treatment planning for liver cancer patients. The proposed approach contributes to precision oncology by enabling reliable, scalable, and data-informed clinical insights, ultimately improving patient management and survival outcomes.

### Keywords:

*Liver Cancer, Artificial Intelligence, Machine Learning, Deep Learning, Survival Analysis, Medical Imaging, Predictive Analytics, Precision Medicine*

## 76. Phytochemical Screening by HPLC and anticancer activity of *Bauhinia variegata* L. bark extracts using HeLa cell line.

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### ABSTRACT

Cancer is the most leading causes of death in world wide. A determined attempts to manage cancers have led to various current treatments including chemotherapy, drugs and radiotherapy, all off which adversely effect on healthy cells of body. The use of alternative herbal medicine has been widely practiced by people worldwide for Cancer treatment. The aim of the study was to analyse the qualitative phytochemical by High performance liquid chromatography for Alkaloid (berberine) in bark extracts of *Bauhinia variegata* L and to determine the anticancer activity of *Bauhinia variegata* L bark extracts against HeLa (human cervical cancer)) cell line, using a standard protocol. It was found that bark extract of *B. variegata* contains phytochemicals that are widely known to have medicinal properties, such as phenols flavonoids, saponins, tannins alkaloids. The Results revealed the presence of berberine in the ethanolic extract of *B. variegata* bark based on retention time of sample as compare with standard berberine. According to the results obtained from the MTT assay, it was observed that when the HeLa cell lines was exposed to different concentrations of the sample. *B. variegata* was found to be cytotoxic effect on HeLa cell line. The present study indicates that *B. variegata* is a potentially strong herbs for anti-cancer agents. The cytotoxic activities of the bark extracts of *B. variegata* can be attributed to the total effects of the phytochemical compounds found. Further studies are needed in order to isolate and determine individual effects of bioactive compounds in *B. variegata*.

**Keywords:** *Bauhinia variegata*, anticancer activity, HeLa cells, phytochemicals, MTT Assay

## 77. Medical 4.0 Technologies for Smart Healthcare Supply Chains

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### ABSTRACT

The rapid evolution of Industry 4.0 has accelerated digital transformation in healthcare systems, giving rise to the concept of Medical 4.0. Medical 4.0 integrates emerging technologies such as the Internet of Things (IoT), artificial intelligence, cloud computing, big data analytics, and blockchain to improve healthcare services and operational efficiency. These technologies play a critical role in transforming the medical supply chain by enabling real-time monitoring, secure data exchange, and improved coordination among healthcare stakeholders. The COVID-19 pandemic highlighted the need for resilient healthcare supply chains capable of ensuring safe distribution of medicines, vaccines, and medical equipment. This study explores the technological ecosystem of Medical 4.0 and its impact on healthcare supply chain management. Through an extensive literature review, the study identifies major technological enablers and their applications in healthcare logistics, including electronic health records, patient monitoring systems, and medication traceability. The research proposes a conceptual framework illustrating how emerging technologies collectively enhance transparency, security, and efficiency in the medical supply chain. The findings indicate that the integration of digital technologies can significantly improve healthcare service delivery while supporting a patient-centric healthcare ecosystem.

*Keywords— Medical 4.0, Healthcare Supply Chain, Digital Healthcare Technologies, Blockchain, IoT, Industry 4.0.*

## **78. Engineering MXene Electrodes with Hydroxide Functionalities for High-Efficiency Supercapacitors**

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### **ABSTRACT**

MXenes have attracted considerable attention as advanced electrode materials for supercapacitor applications due to their excellent electrical conductivity, layered morphology, and tunable surface chemistry. In the present study, hydroxide-engineered MXenes are synthesized and systematically investigated to evaluate their electrochemical energy storage performance. The hydroxide modification is introduced to enhance surface functionality, improve ion diffusion pathways, and stabilize the layered structure of MXenes under electrochemical operation. The structural, optical, and morphological characteristics of the prepared MXene materials are analyzed using UV–Visible spectroscopy, Fourier Transform Infrared (FTIR) spectroscopy, X-ray Diffraction (XRD), and Scanning Electron Microscopy (SEM). The characterization results confirm the formation of well- defined layered MXenes with surface functional groups that promote increased interlayer spacing and improved electrolyte accessibility. Electrochemical properties are primarily examined using Cyclic Voltammetry (CV), Electrochemical Impedance Spectroscopy (EIS), and Galvanostatic Charge–Discharge (GCD) measurements. The CV curves exhibit a combination of electric double- layer capacitance and pseudocapacitive behavior, indicating efficient charge storage mechanisms. EIS analysis reveals low internal resistance and enhanced charge-transfer kinetics, while GCD results demonstrate high specific capacitance, good rate capability, and excellent cycling stability. The improved electrochemical performance is attributed to the synergistic effect of surface engineering, which provides additional active sites and facilitates rapid ion transport. Overall, this study highlights the potential of hydroxide-engineered MXenes as efficient and stable electrode materials for next-generation supercapacitor applications.

*Keywords : MXenes; Hydroxide engineering; Supercapacitor; Electrochemical performance; Energy storage materials*

## 79. Neutrosophic Graphs in Social Network Modeling

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### ABSTRACT

Social networks are fundamental structures for representing interactions among individuals, organizations, and information sources. In real-world scenarios, social relationships are rarely precise; instead, they are affected by uncertainty, incompleteness, inconsistency, and subjectivity. Classical graph-based social network analysis (SNA) methods, which rely on crisp or deterministic edges, are insufficient to model such complex characteristics. This research article proposes a comprehensive framework for social network analysis using neutrosophic graphs, which explicitly incorporate truth, indeterminacy, and falsity components to represent social interactions. By modeling actors as neutrosophic vertices and relationships as neutrosophic edges, the proposed approach captures partial knowledge, contradictory evidence, and missing information within a unified mathematical structure. New formulations of neutrosophic degree, centrality, connectivity, and clustering measures are introduced for social network analysis. The proposed framework is shown to be more flexible, robust, and interpretable than classical and fuzzy graph-based models. Applications to influence analysis, community detection, and opinion dynamics in online social networks are discussed, demonstrating the suitability of neutrosophic graphs for analyzing uncertain and incomplete social data.

### Keywords

*Neutrosophic Graphs, Social Network Analysis, Uncertainty, Indeterminacy, Complex Networks, Neutrosophic Sets, Community Detection, Influence Modeling.*

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