

BOOK OF ABSTRACTS

FOR THE

2nd

INTERNATIONAL CONFERENCE

— ON —

ADVANCED MATERIALS, ENERGY & ENVIRONMENTAL SUSTAINABILITY (ICAMEES 2.0)

Editors

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Organized by
Department of Chemistry,
Applied Science Cluster, SoAE,
UPES, Dehradun



Dec 18-19, 2025



Bidholi Campus, UPES, Dehradun

Message from Chief Patron

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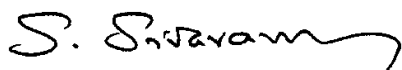
I am happy to note that the Department of Chemistry, Applied Science Cluster, School of Advanced Engineering, UPES Dehradun, is organizing the Second International Conference on Advanced Materials, Energy and Environmental Sustainability (ICAMEES 2.0) on December 18-19, 2025, at Dehradun. ICAMEES 2.0 aims to bring together experts from academia, industry, and research institutions to deliberate on advances in cutting-edge materials and technologies that will propel global energy security and environmental sustainability. The Conference has been organized in three tracks, namely, (1) advanced functional materials, (2) energy harvesting, conversion and storage technologies, and (3) environmental sustainability.

The Conference is both timely and relevant. Advanced functional materials will play a key role in meeting the future challenges around environment and energy, which together constitute the most important pillars of the global sustainability agenda. Several important problems require urgent solutions and, if solved, will have a significant social and economic impact. India faces a unique challenge of combining high economic growth and development with low environmental impact, frugal resource use, and low carbon intensity. We must chart a careful strategy concerning advanced functional materials since many of them are resource-intensive to produce and fabricate.

Research must, therefore, focus on what “needs to be done” rather than “what can be done.” It must address the complexity inherent in such problems, which can be solved only by cross-disciplinary teams. Our higher educational institutions must break the narrow discipline-oriented silos in which they work and forge collaborations, both within and outside the institutions. Every potential solution must be examined through the prism of “sustainability science” to ensure that it does not lead to resource depletion, ecological degradation, and transgression of local, regional, and planetary boundaries.

I hope that this Conference will set aside time to deliberate on a few of these emerging challenges and frame the responses of the scientific community to them. The research community must understand how to factor in holistic sustainability considerations in the design and development of advanced materials, so that we may not commit the mistakes that the earlier generation did, the price of which we are paying today.

I wish the Conference a grand success.



Message from Vice-Chancellor



At UPES, we don't just keep pace with the future - we help create it. I'm delighted to welcome you to the 2nd International Conference on Advanced Materials, Energy & Environmental Sustainability. This isn't a routine event. It's where path-breaking research meets global urgency - where science, technology, and ambition converge.

This past year alone, UPES surged over 800 positions in the QS Sustainability Rankings, now standing at 682 globally - a testament of our relentless commitment to meaningful, measurable change. In the latest QS Asia University Rankings, we're 24th in South Asia, and in Engineering & Technology, we are now counted among the world's top 250. These are not just accolades; they are the result of tireless effort from our faculty, students, and partners focused on research that matters and impact that lasts.

ICAMEES 2.0 brings together brilliant minds from across disciplines and continents. This is your space to think differently, challenge each other, and build ideas that travel far beyond the university gates. Thank you for joining us.



(Prof. Ram Sharma)

Message from Dean, R&D



With great pleasure I extend my heartfelt congratulations to the Department of Chemistry, Applied Science Cluster of the School of Advanced Engineering, UPES, for organizing the 2nd International Conference on Advanced Materials, Energy & Environmental Sustainability (ICAMEES 2.0) scheduled for December 18-19, 2025 at UPES, Dehradun. This conference exemplifies UPES's unwavering commitment to fostering research, innovation, and interdisciplinary collaboration to address solutions for urgent global challenges in engineering and environmental sustainability. By focusing on cutting-edge advancements in various types of materials, energy harvesting and storage, and environmental protection, the conference will address critical areas such as climate science, renewable energy, and environmental sustenance. The conference themes underscore the essential role of chemical sciences and innovations in driving sustainable solutions to global challenges.

I extend my best wishes to the organizers, participants, and stakeholders for a successful and impactful conference. May ICAMEES 2.0 inspire groundbreaking solutions, foster lasting collaborations, and pave the way for a sustainable and resilient future.

A handwritten signature in black ink, appearing to read 'Ashwini Nangia'.

(Prof. Ashwini K. Nangia)

Message from Cluster Head



It is my privilege to welcome you to the 2nd International Conference on Advanced Materials, Energy & Environmental Sustainability (ICAMEES 2.0) from December 18-19, 2025.

I am delighted to see that ICAMEES 2.0 unites luminaries from academia, research, and industry, exploring cutting-edge advancements in chemical sciences with a special emphasis on advanced materials and their applications in energy and environmental sustainability. This conference delves into critical areas such as different categories of materials, energy resources, energy harvesting and storage, and various aspects covering environmental sustainability, fostering interdisciplinary collaborations to address pressing global challenges.

Through keynote talks, invited lectures, and expert discussions, ICAMEES 2.0 provides a vibrant platform for exchanging ideas, sparking innovation, and forging partnerships. Your contributions will be instrumental in advancing the frontiers of chemical sciences and shaping sustainable solutions for the future.

We are privileged to host this event in Dehradun, a serene city nestled in the foothills of the Himalayas, renowned for its picturesque landscapes and vibrant academic ecosystem. In December, Dehradun offers a cold weather, with relatively lower temperatures with calmness and serenity, making it an ideal setting for intellectual exchange and exploration.

I extend my heartfelt gratitude to the organizing committee for their tireless efforts, the distinguished speakers, and all participants who are contributing to the vibrant discourse. Your presence will undoubtedly make ICAMEES 2.0 a landmark event in advancing chemical sciences for a sustainable future.

(Prof. Ranjeet K. Brajpuriya)

Message from Convener



It is an honour and pleasure to extend warm welcome to all the delegates, invited and plenary speakers to the 2nd International Conference on Advanced Materials, Energy & Environmental Sustainability (ICAMEES 2.0) being organized by Department of Chemistry, Applied Science Cluster, School of Advanced Engineering at UPES, Dehradun (India).

The aim of the conference endeavours to address wide ranging issues from synthesis and characterization of advanced materials for energy production & storage to environmental sustainability through various unique approaches.

I am confident that the deliberations and interactions in this event will lead to development of strategies, not only for impact assessment but also for advancement in exploring applications in various dimensions of life and society. I look forward to different user communities being benefited from ICAMEES 2.0, envisioning it as an opportunity to promote and document the recent developments in the fields of materials science, energy and environment; meet experts from a wide range of fields and developing new collaborations; and exchange technical/scientific information with various industries and R&D organizations.

I perceive ICAMEES 2.0 as a prospective platform for all the participants from across the globe and wish them a pleasant and memorable stay at Dehradun.

A handwritten signature in black ink, appearing to be 'S. Singhal'.

(Prof. Shailey Singhal)

Preface

We are delighted to present the Abstract Booklet for the second edition of the International Conference on Advanced Materials, Energy & Environmental Sustainability (ICAMEES). Building on the success and encouraging response of our inaugural conference, and the continued enthusiasm from the academic and professional community have inspired us to bring this platform back with renewed purpose and broader vision.

The second edition of this conference reaffirms our commitment towards nurturing a vibrant space for knowledge exchange, innovation, and critical inquiry. The abstracts compiled in this volume represent a depth, diverse range of perspectives, and evolving nature of research being undertaken across various domains. Each contribution reflects the curiosity, rigor, and dedication of scholars and practitioners who strive to address contemporary challenges and advance their fields.

Organizing this conference for the second time is not merely a continuation—it is a step forward in strengthening collaboration, fostering interdisciplinary dialogue, and building a sustained culture of shared learning. We extend our sincere appreciation to all contributors for sharing their work, reviewers, session chairs, and members of the organizing committee for their dedication, and to all participants for their enthusiasm and support. We also thank all participants for their active engagement and support.

We hope that the discussions sparked here will inspire new ideas, meaningful partnerships, and future pathways for research and innovation.

We wish all delegates a productive and intellectually enriching experience.

(Organizing Committee)

Department of Chemistry,
Applied Science Cluster, SoAE
UPES, Dehradun

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Plenary Talk

Sustainability and Circular Economy Initiatives in Indian Cement Industry

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In the fast growing infrastructure of our country, use of sustainable materials is the key in the circular economy. Environment-friendly materials (also known as green building materials) are those in which, for their production, placing and maintenance, actions of low environmental impact have been performed. They have to be durable, reusable or recyclable. These materials also have to be natural and must not be spoilt by cold, heat or humidity. Concrete is the most widely used man-made material on earth and approximately, 2.0-2.5 m³ of concrete person is used. Though concrete is not a natural material but due to its superiority features it's a material of choice for infrastructure development. It forms the foundations of cities and connects communities and without it, many of the elements of modern life wouldn't be possible. The basic ingredient of concrete is cement and 7-8% of total CO₂ emission in the world is by the cement production only. Due to the increasing concerns of climate change, cement industries are on the radar of policy makers to lower their carbon foot-prints. Cement industries have been asked to be carbon neutral by 2050. There is a significant challenge involved in achieving sustainability by cement industry. India is the second largest producer of cement after China and therefore, to meet the target of 2050 innovative indigenous efforts are required. The present talk will provide an overview of the Research & Development efforts being undertaken in achieving the concrete sustainability.

Keynote Talks

Tetrapods based Advanced Materials for Advanced Technologies

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Considering the size dependent utilization complexities of nanoscopic dimensions in real technologies, the focus of nanomaterials community is converging to three-dimensional (3D) smart nanomaterials which are built out of interconnected nanostructures building blocks. This talk will briefly introduce the importance of tetrapod nanostructures towards smart 3D ceramic nanostructuring via a simple and single step flame-based approach for synthesis of zinc oxide tetrapods. These ceramic tetrapods have already demonstrated their potential roles in many different technologies. These zinc oxide tetrapods can be used as solid backbone or sacrificial templates to design hybrid or new tetrapods as smart materials. These smart 3D nanomaterials offer many applications in engineering and advanced technologies. Application examples of 3D ceramic tetrapods in nanosensing, optical sensing, whispering gallery mode resonances, light trapping and guiding, composite engineering, antiviral candidates, water purification, piezotronics, agriculture, and in several other applications will be demonstrated [1-10]. The integration of tetrapods in electrospun fibers offer many advantages in biomedical engineering and few examples about nano-engineered electrospun fibers will be presented as recent developments.

Keywords: Zinc Oxide Tetrapods, Smart Materials, Advanced Technologies

References:

1. *Small*, 2025, **21**, 2408414.
2. *Materials Today Electronics*, 2024, **8**, 100102.
3. *Chemical Engineering Journal*, 2023, **462**, 141984.
4. *Progress in Materials Science*, 2023, **139**, 101169.
5. *Progress in Polymer Science*, 2022, 101516.
6. *Materials Today*, 2021, **50**, 533-569.
7. *Materials Today*, 2021, **48**, 7-17.
8. *Advanced Functional Materials*, 2021, **31**, 20007555.
9. *Materials Today*, 2020, **32**, 108 -130.
10. *Materials Today*, 2018, **6**, 631-651.

Creating Circularity and generating Value out of Single Use Waste Plastic

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Plastics are ubiquitous but have become a victim of their own versatility. Plastics, in many ways, contribute positively to society and it is not possible to imagine a life without plastics today. There is, however, a dark side: the way we produce, use and dispose of plastics is polluting ecosystems, creating risks for human and animal health and destabilizing the climate. India's plastic consumption has reached more than 22 Mnt (Million tons) in 2023 and growing at 8-9%. India's plastic market is about 3.5 Lakh Crore i.e. approx. 42 Bn USD. This is expected to increase to 10 Lakh crore by the next 5-years. At the same time, India's plastic waste output has increased substantially over the years. While India produced about 4.2 Mnt of plastic waste in 2023, only 30% of it is recycled, and the rest of the plastic waste is sent to landfills or aquatic dumps.

Alarmed by the adverse impact of plastic waste story, the plastics industry world over is striving to transform the traditional linear economy-where plastics are typically disposed of at the end of their service life-into a plastics circular economy. The plastics circular economy is a sustainable model where plastics remain in circulation longer and are reused and recycled at the end of their life span.

This talk shall cover several technical pathways to create value out of Single Use Waste Plastic for various stakeholders right from rag pickers, waste handlers, aggregators, processors and converters etc. The technology pathways utilize three prong approaches of Mechanical Recycling, Chemical Recycling and Biological Recycling of waste plastic materials. Several case studies and examples around each technical pathways shall be presented, For example, creating an effective After-Use Plastic Economy by utilizing such waste plastic in existing refineries, converting waste plastic to value added chemicals, upcycling of single use plastic into valuable products, utilizing waste plastic for road pavement/paver blocks etc, along with value proposition by each of the pathways. Further the talk shall discuss the emerging field of Biodegradable/Bio-based Plastics, besides impediments to the implementation of such technologies at large scale.

Crafting Startup Success Stories for A Sustainable Future within India

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Two metrics—materials resource efficiency and energy efficiency—can adequately encompass most key imperatives for a sustainable planet. Startups in India offering climate-oriented technologies need to align with these metrics. They must also demonstrate the ability to drive globally benchmarked, yet locally meaningful, technology outcomes backed by evidence-based science and robust, sustainable supply chains. The large body of academic knowledge within India, coupled with the widespread availability of data analytics, machine learning and artificial intelligence toolkits, offers significant opportunities to emerging companies. Case studies related to lubrication, corrosion and building energy management are discussed.

Invited Talks

Asymmetric Synthesis of Chiral Compounds from CO₂ at Chiral Encoded Metal Surfaces

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The design of chiral surfaces is one of the most crucial topics in modern chemistry, particularly in catalysis as they can be used to selectively produce chiral compounds, which can exhibit a positive effect on biological activity for one enantiomer, whereas the other one even shows toxicity. Previously, we have successfully designed chiral encoded Pt-Ir alloys which showed excellent performance as both electrocatalysts and heterogeneous catalysts for asymmetric synthesis of chiral model compounds via either electroreduction or hydrogenation of prochiral molecules¹⁻³. To extend the applications of chiral encoded Pt-Ir electrocatalysts, we report in this contribution a novel strategy for the enantioselective electrochemical synthesis of chiral compounds, such as mandelic acid enantiomers (*R*-MA, *S*-MA) from carbon dioxide (CO₂). In this case, chiral mesoporous Pt-Ir alloys, imprinted with mandelic acid enantiomers, were prepared by the electrodeposition from Pt and Ir salts in the simultaneous presence of non-ionic surfactants, and mandelic acid enantiomers, which were used as mesoporegens and chiral templates, respectively. After electrodeposition, both, surfactants and chiral templates were removed completely. The cleaned electrodes have been characterized by enantioselective recognition tests of the corresponding chiral compounds by Differential Pulse Voltammetry (DPV). It was found that when using the chiral mesoporous Pt-Ir imprinted with *R*-MA, higher currents are recorded in the presence of *R*-MA compared to the other enantiomer, and vice-versa when using the one imprinted with the opposite stereoisomer.

Most importantly, the chiral imprinted Pt-Ir alloys deposited on nickel foam were then applied as electrocatalysts for the electrocarboxylation of benzaldehyde with CO₂ at 4°C. When using pulse electrosynthesis, an enantiomeric excess (*ee*) of approximately 50 % was obtained for synthesizing the respective mandelic acid enantiomers. However, the mechanical stability of these materials when using nickel foam as the conductive support material is still limited. To further improve the stability, carbon felt was used instead of nickel foam. Interestingly, a high enantiomeric excess (*ee*) of approximately 40 % was observed when using chiral encoded Pt-Ir alloys deposited on carbon felt as working electrodes, even when reusing them for several catalytic cycles. This first example illustrates a novel concept for the asymmetric synthesis of chiral compounds using chiral encoded metals as electrocatalysts for electrocarboxylation[4].

References

1. S. Assavapanumat *et al.*, *J. Am. Chem. Soc.*, 2019, **141**, 18870.
2. S. Supattra *et al.* *Chem. Eur. J.*, 2023, **29**, e2023020.
3. S. Butcha *et al.* *Nat. Comm*, 2021, **12**, 1314.
4. A. Sohail *et al.* (*manuscript in preparation*).

Potentiodynamic Actuation of Carbon Fibers

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Shape-changing structures have broad potential applications,¹ but they often require tailored modifications.² In this work, we present a simple and direct approach to actuating carbon fibers in a bipolar electrochemical cell³ by inducing asymmetric reactions along the surface grooves of the fibers.⁴ A carbon fiber mounted in the partition of a sealed bipolar electrochemical cell is polarized to trigger asymmetric redox reactions of benzoquinone and hydroquinone in two separate compartments. Once the threshold potential is exceeded, ion adsorption occurs, and the fiber segment involved in the anodic reaction undergoes reversible, directional motion. Elemental surface analysis of the polarized fiber reveals that this bending arises from ion intercalation and deintercalation accompanying the oxidation and reduction of the fiber surface. Simultaneous local ion adsorption and desorption drive the deflection of the fiber. The length of the fiber in the opposite compartment, where electroreduction takes place, together with the orientation of the grooves, governs the amplitude and direction of motion. Optimal fiber alignment and excitation voltage yield efficient bending, while actuation of two parallel, oppositely oriented fibers produces a motion resembling a micro-tweezer.⁵ We anticipate that these findings will expand the toolkit for research in microrobotics and micromechanics.

References

1. L. Kong *et al.*, *Adv. Mater.*, 2014, **26**, 1025.
2. A. A. Melvin *et al.*, *Adv. Funct. Mater.*, 2021, **31**, 2101171.
3. G. Loget *et al.*, *Acc. Chem. Res.*, 2013, **46**, 2513.
4. B. Gupta *et al.*, *Nat. Commun.*, Accepted (2025).
5. K. C. Johnson *et al.*, *J. Biol. Eng.* 2017, **11**, 47.

R&D Initiatives in CBRN Defence Preparedness: New Hopes in Hybrid Warfare

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The evolving landscape of Chemical, Biological, Radiological and Nuclear (CBRN) threats necessitates sustained and innovative research and development (R&D) efforts to strengthen national defence preparedness. Current initiatives focus on developing advanced detection, protection, and decontamination technologies that enable rapid response and mitigation during CBRN emergencies. Key research domains include real-time sensing systems using nanomaterials and AI-enabled analytics, next-generation personal protective equipment (PPE) with enhanced filtration and ergonomic performance, and high-efficiency decontamination formulations tailored for chemical agents, biological contaminants, and radionuclides. Parallel efforts aim at modelling dispersion patterns, risk assessment frameworks, and decision-support tools to support evidence-based emergency management. Integration of indigenous material science, biotechnology, and nuclear instrumentation research with operational needs ensures the development of robust, cost-effective, and field-deployable solutions. Collectively, these R&D initiatives contribute to a comprehensive and resilient CBRN defence architecture, enhancing national capability for prevention, detection, response, and recovery in the face of emerging threats.

Tuning the Magnetic State in Transition Metal Oxides Thin Films via Strain

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Strain engineering in thin films of transition metal (TM) oxides materials provides a window to tune the TM 3d-O 2p hybridization as well as charge transfer energy, which control their electronic and magnetic ground states. However, generally strained films also suffer from other defect states, such as oxygen vacancy, local distortion etc. and hence it is difficult to conclude the origin of modification in the physical properties in such films. It is of huge importance and fundamental in nature to ascertain an unequivocal origin of modifications in electrical, electronic and magnetic properties, in order to tune their properties. I shall discuss some of our recent results on inducing different types of strain in transition metal oxides based materials and its consequences on its electrical, electronic, structural and magnetic properties.

Innovative Chemistries for the Development of Sustainable and Eco-Friendly Additives

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Traditional lubricant additives have negative effects on the environment during manufacture, usage, and disposal. In addition, regulatory constraints and machine performance issues like incompatibility with the new engine materials must be addressed. Therefore, the development of new additions is a major priority in order to fulfil the increasing demands and environmental difficulties caused by the traditional chemicals used in the petroleum business. This talk will concentrate on outlining the most recent advancements in environmentally acceptable alternatives. The many potential strategies will be briefly discussed. I'll also give an overview of some of the most intriguing and cutting-edge R&D developments in the additive industry that are based on sustainable biomaterials.

Catalysis, Sensing and Phytofabrication of Metallic Nanoparticles: From Green Synthesis to Environmental Remediation

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The green synthesis of nanoscale materials is of special interest to researchers all over the world. We describe a simple, robust, inexpensive, and environmentally friendly approach to the synthesis of gold, silver, copper and iron oxide nanoparticles using a variety of biomolecules/ phytochemicals as potential reducers and stabilizers. The green approach to the controlled synthesis of nanoparticles with different morphologies is based on the use of plant extracts. In this lecture, current plant-mediated strategies for preparing nanoparticles of gold, silver, and iron are briefly described, and morphologically dependent nanoparticles for the antioxidant activity, H₂O₂ sensing, catalytic activity for the remediation of organic pollutants are highlighted. Overall, the approach presented in the article supports environmental protection and is a promising alternative to other synthesis techniques.

References

1. B. Kumar *et al.*, *Inorg. Chem. Commun.*, 2021, **133**, 108868.
2. B. Kumar *et al.*, *Chem. Phys. Lett.*, 2021, **781**, 138993.
3. B. Kumar *et al.*, *J. Compos. Sci.*, 2021, **5**, 219.
4. B. Kumar *et al.*, *Waste Biomass Valori.*, 2021, **12**, 3575.
5. B. Kumar *et al.*, *Bioeng.*, 2020, **7**, 54.

Transforming Natural Clays into Functional Porous Materials for Sustainable Air, Water, and Bioenergy Purification Technologies

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Natural clays represent abundant, low-cost, and environmentally compatible resources that can be transformed into high-performance adsorbents through targeted structural modification and interlayer engineering. Our research efforts over the past several years have focused on developing pillared clays, porous clay heterostructures, and clay–carbon composites, where textural properties, pore connectivity, and surface chemistry are systematically enhanced to improve adsorption selectivity. Using metal-pillaring, surfactant-assisted structuring, and organic modification approaches, we have demonstrated significant improvements in the ability of these materials to address key environmental purification challenges. In the area of air quality management, modified montmorillonite systems exhibit strong affinity and selectivity for indoor VOCs (BTEX) and enable efficient CO₂ removal for biogas upgrading, as reported in our recent studies on Al- and Zr-pillared clays and PCH materials. For water purification, modified clay materials and clay–carbon composite beads show excellent capabilities in removing emerging organic pollutants, pharmaceuticals, pesticides, and other harmful chemicals. By correlating pore architecture, surface chemistry, and adsorption mechanisms, our work highlights how natural clays can be upgraded into functional porous materials with tunable performance. This presentation will consolidate these advances to demonstrate how sustainably engineered clay-based materials can provide scalable, energy- efficient solutions for both air and water purification technologies, contributing to the broader goal of environmental sustainability.

Catalyst-Free Construction and Photophysical Analysis of Base-Modified Fluorescent Nucleosides

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Fluorescent nucleosides, engineered by substituting natural nucleobases with luminescent analogues, have become essential molecular tools for elucidating nucleic acid structure, dynamics, and interactions. Strategic chemical modifications endow these probes with optimal photophysical features, while faithfully preserving the base-pairing capacity needed for DNA and RNA functionality. This design enables real-time tracking of molecular events and renders these nucleosides highly sensitive to diverse microenvironmental changes, such as shifts in polarity or protein association, greatly expanding their utility in diagnostic assays, high-throughput screening, and live-cell imaging applications.

In the present study, novel fluorescent nucleosides bearing diverse heterocyclic scaffolds at the C-5 position of uridine were systematically designed to achieve both improved emission efficiency and synthetic practicality. Utilizing a catalyst-free, atom-economical multicomponent synthetic approach, oxazine-coumarin triazoles, furo[3,2-c]coumarins, 1,4-dihydropyridines, and furo[3,2-c]quinolones were incorporated into nucleoside frameworks. Detailed characterization of their photophysical properties revealed that precise integration of heteroaromatic motifs considerably amplifies fluorescence and unlocks new directions for applications in nucleic acid chemistry and molecular diagnostics.

Keywords: Base-Modified, Nucleosides, Fluorescent, Photophysical, Pyridine/Thymine

References

1. Arora *et al.*, *Org. Biomol. Chem.*, 2024, **22**, 4922.
2. S. Kumar *et al.*, *J. Mol. Struct.*, 2025, **1321**, 139915.
3. Arora *et al.*, *RSC Adv.*, 2024, **14**, 39833.
4. S. Kumar *et al.*, *Dyes Pigm.*, 2025, **240**, 112826.

Structural understanding and modification of biomacromolecules using green chemistry

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Nature continues to provide amazingly diverse biomacromolecules including polysaccharides for varied applications. Structural analysis of these polysaccharides is a critical prerequisite towards understanding the functional properties, structural activity and subsequent modification for commercial utilization. Therefore, a series of polysaccharides including complex arabinoxylans comprising the backbone of $\rightarrow 4$)- β -D-linked Xylp(1 \rightarrow with branching at O-2 by $\rightarrow 3$)- α -L-Araf(1 \rightarrow and $\rightarrow 3$)- β -D-Xylp(1 \rightarrow chain; arabinogalactans having 1,4-linked 3-O-methyl- β -D-galactopyranose and β -D-galactopyranose backbone with branching at O-6 of 3-O-methyl- β -D-galactosyl residues by 1,5-linked 3-O-methyl- α -L-arabinofuranoside chains. etc. were thoroughly analyzed by advanced separation and spectroscopic (^1H , ^{13}C , ^1H - ^1H -COSY, HSQC, HMBC) methods.

Intriguingly, several polysaccharides proved to be inadequate in specific end-use properties due to fixed molecular weight and constitution. Accordingly, galactomannans have been crosslinked using green chemistry approach in our laboratory. The synthesized biomaterials demonstrated controlled drug delivery making them potential candidates for pharmaceutical and biological applications. Developing such green formulations from abundant biomacromolecules using green chemistry methods offers myriad benefits, stimulating future studies on biomass conversion to biomedical products, thereby, benefiting both humans and the environment. The lecture will highlight the chemical modifications done, patents filed and technologies developed/being developed to prepare biomaterials for the benefit of society.

Keywords: Biomacromolecules, green chemistry, biomaterials, polysaccharides, NMR

Graphene Oxide a Promising Adsorbent for Water Remediation and Enhancing Water Portability

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Improving the water quality by reducing pollution is an important sustainable development goal (SGDs-6) of UNEP program which is aimed to provide quality water for future generations. Application of materials science-based solutions are gaining importance, particularly designing and development of porous, high surface area materials and inexpensive and reusable materials for removal of water pollutants and to improve water quality for drinking and other domestic purposes. An important constraint in water purification is presence of pollutants such as toxic metal ions (As, Ca, Hg, Pb), fluorides, synthetic dyes, carcinogenic PAHs in quite low concentrations, i.e., ppb-ppm range. To remove such low-level of pollutants requires two-dimensional (2D) graphene materials with unique properties - high surface area, ease in functionalization, high stability in harsh conditions and reusability – are very much needed in the current scenario of water quality improvement programs. In our study, plastic wastes, sludges and graphite raw materials were used to prepare few-layered graphene (FLG) by hydrothermal processes, this waste utilization reduces environmental burden of plastic wastes and sludges. The graphene yields achieved 36-42% using solid wastes (plastic waste and sludge) and few-layered graphene materials showed surface area between 1220 – 1360 m²/g and predominate carboxylic acid, hydroxyl, ketonic functionalities favourable for adsorption of traces of water pollutants. The adsorption mechanism predominated by electrostatic interaction and π - π stacking while adsorption metal ions favoured coordination bonding. The adsorption removal of water pollutants followed the pseudo-second-order kinetics and the non-linear Langmuir isotherm. The FLG have shown reusability about 20 cycles and for washing of spent FLGs dilute HNO₃ (0.01 N) reported as economically viable option. The adsorption removal of water pollutants by different adsorbents was compared with the FLG prepared and applied in this study for water purification was discussed.

Digital Therapeutics (DTx): Transforming Healthcare Through 21st Century Innovation

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As the digital era accelerates, global adoption of advanced technologies is fundamentally reshaping the healthcare landscape. Healthcare systems are undergoing transformative changes due to innovative technology solutions which enable a shift towards a more data-driven and personalised model of healthcare. In this dynamic environment, the pharmaceutical sector stands out as a highly regulated industry which consistently strives to protect public health while maintaining a steadfast commitment to patient-centric innovations. Digital Therapeutics (DTx) have emerged as a groundbreaking field at the intersection of technology with medicine for offering evidence-based therapeutic interventions delivered through software and digital platforms. DTx enable patients and providers to access high-quality treatment options that complement or have the potential to replace traditional therapies at a certain level.

As countries begin to implement DTx, regulatory authorities, including national and international levels, are closely monitoring potential risks, benefits and implementation challenges. The regulatory approaches and management strategies adopted in one region have significant potential policies and practices globally, which underlie the necessity for international cooperation. The rise of DTx is prompting a re-evaluation of existing healthcare regulations and is opening doors to novel therapeutic possibilities. There is now a need to address the fundamental principles, practical application, and regulatory framework that underpin DTx, as they act as a bridge to the traditional gaps between technology and medicine. Policymakers and industry leaders must prioritise the development of harmonised forward-thinking regulatory strategies to ensure that DTx are able to deliver on their promise of safer, more effective and widely accessible healthcare solutions for all.

Role Of Educational Institutes in Climate Change and Circular Economy- A Step Towards Net Carbon Zero Mission

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India G20 presidency India privatized sustainable development and climate change. At the Voice of the Global South Summit convened by India, GOI spoke for the need for climate action based on the principles of equity, climate justice and common but differentiated responsibilities, as well as a greater focus on adaptation. As per GOI mission, it is important that the efforts of the developing world be supported with adequate climate financing and technology transfer. They must have access to equitable carbon and development space to achieve sustainable development.

Renewables offer a way out of import dependency, allowing countries to diversify their economies and protect them from the unpredictable price swings of fossil fuels, while driving inclusive economic growth, new jobs, and poverty alleviation. Renewable energy actually is the cheapest power option in most parts of the world today. Falling prices make renewable energy more attractive all around – including to low- and middle-income countries, where most of the additional demand for new electricity will come from. Switching to clean sources of energy, such as Biofuels, wind and solar, thus helps address not only climate change but also air pollution and health. Every dollar of investment in renewables creates three times more jobs than in the fossil fuel industry.

The IEA (International energy agency) estimates that the transition towards net-zero emissions will lead to an overall increase in energy sector jobs, resulting in a net gain of 9 million jobs. The reduction of pollution and climate impacts alone could save the world up to \$4.2 trillion per year by 2030. Moreover, efficient and reliable renewable technologies can create a system less prone to market shocks and improve resilience and energy security by diversifying power supply options. Further, an educational Institute and Universities need to play indispensable as well as key role towards Net carbon zero mission to fulfill SDG 7 & 13 Goals for circular economy.

Contribution of Chemistry in Advancing the Sustainable Development Goals

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Chemistry plays a pivotal role in advancing the development of a sustainable society and in achieving the United Nations Sustainable Development Goals (SDGs). As an indispensable branch of science, chemistry necessitates continuous refinement to enhance environmental protection, optimize resource utilization, and minimize waste generation. The synthesis of both simple and structurally complex organic molecules remains fundamental to chemical science domain. The principles of green chemistry redesign traditional synthetic methodologies leading to reduction in their ecological footprint while maintaining or improving efficiency and selectivity. Strategies such as the employment of catalysts, improved atom economy, solvent-free or alternative solvent systems, and the utilization of renewable feedstocks contribute significantly to the development of cleaner and safer chemical processes. The present discussion will elaborate on selected sustainable approaches and their respective environmental advantages in detail.

Oral Presentations

Fe-Zr Mofs as an Effective Adsorbent for Cr(VI) Removal from Aqueous Solution

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Here, the metal-organic frameworks (MOF) of Iron and zirconium (Fe-Zr) were prepared and used for the removal of Cr (VI) from aqueous solution. The Fe-Zr MOFs formation was confirmed with FESEM, FTIR, Raman, and XRD instrumental techniques. In the optimum condition of pH 3, concentration of Cr (VI) ion 20 mg/L, the Fe-Zr MOFs were able to remove 95% of Cr(VI) from aqueous solution. The adsorption process followed the Langmuir isothermal adsorption model. The chemisorption nature of the adsorption process was confirmed by the second-order kinetic model. The adsorption process was spontaneous and heat-absorbing, as confirmed from thermodynamic analysis. The material regenerated with a 0.1M NaOH solution and can be used up to five cycles without any decrease in efficiency. The possible adsorption mechanism suggested that electrostatic attraction, pore diffusion, reduction, and chemical coordination were going on between Cr(VI) and Fe-Zr MOFs, respectively. The Fe-Zr MOFs can be potentially applied to real wastewater containing Cr(VI).

Synthesis, Micellization and Morphological Behaviour of Cholesterol-based Conventional and Gemini Surfactants in Deep Eutectic Solvent (ChCl: EG)

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Cholesterol based conventional cationic surfactants (Chol-DMG, Chol-DMPA, Chol-DMBA and Chol-DMABA) & Cationic Gemini surfactant (Ch-4-Ch) have been synthesized, via multiple steps. The synthesized surfactants were characterized by Fourier-transform infrared (FTIR), proton nuclear magnetic resonance (^1H NMR) spectroscopy, and Elemental (CHN) Analysis. Physico-chemical properties (micellization, surface parameters, etc.) have been examined by surface tension measurement in Deep Eutectic Solvents (DES, Choline Chloride + Ethylene glycol). The study revealed that cholesterol-based surfactants shown better micelle formation, improved surface arrangements in the presence of DES. Mixed micellization and Morphological characterization have been performed of cationic conventional (cholesterol based) and anionic (SDS/SDC) surfactants using techniques such as viscosity, refractive index, dynamic light scattering (DLS), Zeta Potential, transmission electron microscopy (TEM). This work offers a new information for the use of biocompatible surfactants with desired properties to potential biomedical applications, drug delivery, gene transfection, bio-imaging, etc.

Novel Dendritic Oligomeric Surfactants: Theoretical and Practical Approaches

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Dendritic oligomeric cationic surfactants (DOS, 3C12tri, 4C12tetra and 6C12hexa, contains three, four and six hydrophobic chains and charged hydrophilic headgroups connected by amide-type spacer groups) were synthesized and characterized (NMR, FT-IR, CHN, and ESI-Mass). Micellization (CMC, Krafft temperature), surface parameters, micro-polarity environment and surface arrangement of DOS were investigated by using surface tension, electrical conductivity, steady-state fluorescence and 2D NMR measurements, respectively. Morphological (higher order aggregates) behaviour of DOS along with anionic surfactant (Sodium deoxycholate, SDC) were analysed using zeta-potential, DLS, TEM, etc. To understand the molecular properties like HOMO–LUMO energy gap, electron cloud, EPT, and binding properties of these newly synthesized DOS, stimulation dynamic studies were performed thoroughly. This study will use to understand the pure and mixed monomeric arrangement in aqueous solution to enhance the applicability.

Encapsulation and Released of Piperine or Curcumin: An Effect of Surfactant Formulation

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Bioactive compounds (such as Piperine and Curcumin) offer a notable pharmacological advantage. Nonetheless, their clinical use is hindered by their poor solubility in water and limited bioavailability. This study explores the use of surfactant-based different morphological systems, which include pure and mixed conventional, gemini and dendritic oligomeric surfactants, to improve the encapsulation, stability, and bioavailability as well as their release profile of the bioactive compounds. The encapsulation and release study were measured quantitatively through UV-Visible spectroscopy. The findings indicated a significant enhancement in the solubility of Piperine and Curcumin with higher concentrations of surfactants, underscoring their role in increasing water solubility. Additionally, higher order of aggregates provides a more favourable environment for the encapsulation of bio-moieties compared to micellar aggregates. Ultimately, the research highlights the potential of micellar systems as effective delivery methods to enhance the therapeutic application of hydrophobic herbal bioactive.

Role of Aromatic Interactions in Disassembly of Biotinylated Ditryptophan Nanostructures

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Biotinylated ditryptophan short peptide has been studied to form spherical self-assembly in aqueous-organic solvents but as soon as an aromatic solvent such as benzene is added to the solution, we observed the disassembly of spherical nanostructures. Spectroscopic and microscopic studies conformed this morphological change which was due to aromatic interaction but this aromatic interaction disturbs the intermolecular aromatic stacking between peptide molecules and led the disassembly of peptide nanostructures. Such kind of morphological disassembly of peptide nanostructures can be used for the targeted drug delivery where disassembly of peptide will lead to the release of desired drug molecules and noble metal nanoparticles. It may attract scientific interest in the field of medicinal chemistry, drug delivery and nanotherapy.

Facetted Nano-assemblies of Tryptocidine C, a tryptophan-rich Cyclic Decapeptide with Antimicrobial Activity

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A Trp-rich cyclodecapeptide, tryptocidine C (TpcC) has been previously been shown to oligomerize in solution and form small nanospheres with a 24 nm diameter, large nanospheroids and facetted 3-D crystals when dried from ethanolic solutions. In this study we assessed the self-assembly of TpcC dried from a 50% acetonitrile:water (v/v) solution using high-resolution scanning electron microscopy (SEM), scanning transmission electron microscopy (STEM) and atomic force microscopy (AFM). From the STEM, SEM and AFM analysis of TpcC in 50% acetonitrile it was deduced that small nanospheres, similar to those previously observed, pack into larger oblate TpcC nanospheroids. Detailed analysis of SEM data using a novel Mathematica algorithm revealed the bulk of the nanospheroids have a diameter of 246 ± 50 nm, notably with the same low polydispersity (0.04) as previously found for the small nanospheres. Further analyses revealed that the large nanospheroids increase in density with time by attracting more TpcC monomers/oligomers. The small TpcC nanospheres and sheet-like structures act as a feedstock, from which facetted 3-D TpcC crystals can grow. From a non-crystallographic approach, we propose sheet- and small nanospheres as feedstock for the three-dimensional packing of the small TpcC nanospheres that form larger 3-D TpcC icosahedrons leading to different facetted crystals. The small population of these larger structures in 50% acetonitrile over time did not impede the surface derived antimicrobial activity, as the bulk of active peptide remained metastable structures, probably existing as sheets and small nanoparticles.

Keywords: Antimicrobial cyclic peptide, tryptocidine, tyrothricin, self-assembly, nanocrystals, morphology, antimicrobial activity, surface activity.

Performance Analysis of Concrete-Based Solar Energy Flat Collector for Water Heating

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The easiest and advantageous way to acquire useful energy is to simply convert what is available in nature into more useful forms. This review work with the purpose on the theme “Energy Harvesting and Storage” is focused on Concrete-based solar collectors, due to their low cost, durability, and inherent thermal storage capacity, are emerging as viable alternatives to conventional flat plate collectors for water heating. This review study presents a detailed performance analysis of a concrete-based solar water heating system by examining key influencing parameters such as water mass flow rate, collector inclination, pipe diameter and material, spacing between flow pipe in concrete, flow pipe pattern and its arrangement, azimuth angle and mixing of metal scraps in concrete to improve its thermal conductivity to enhance the solar absorption in storage system. Reviews of experimental observations and analytical modelling indicate that lower mass flow rates yield higher outlet temperatures in range of 60°C but at the expense of reduced overall efficiency, while optimized flow rates balance both parameters. Similarly, variations in collector inclination and azimuth angle strongly affect solar energy absorption, with maximum efficiency achieved when the collector is oriented to minimize angular losses relative to incident solar radiation. Space between two fluid carrying pipes influence the thermal resistance and fixed this space as 6 cm optimum. The study highlights the potential of integrating concrete as both an absorber and storage medium, providing a cost-effective, sustainable, and thermally reliable solution for domestic hot water applications with fluid carrying pipe diameter of 19 mm and concrete thickness in range of 5 cm.

Covalent Organic Framework Square Lattice for High Performance Supercapacitor

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Covalent Organic Frameworks (COFs) are a promising materials for next generation energy conversion and storage. COFs are a class of porous materials where the organic ligands (struts) are connected each other to form a crystalline and long range periodic network. The presence of structural periodicity and open pores, they can be used for ion transport and storage applications. Depending on the size and length of the struts, this pore can be tuned and functionalized as per the requirement. Here, we have designed a porphyrin based PT-COF where the C_2 symmetrical aromatic aldehyde, [1,1,2,2-tetrakis(4-formyl-(1,1'-biphenyl))-ethane] (TFBE) and C_4 symmetrical aromatic amine, 5,10,15,20-tetrakis-(para-amino phenyl) porphyrin (TAPP) were used for solvothermal synthesis of PT-COF. The COF shows very high surface area of $1998 \text{ m}^2 \text{ g}^{-1}$ with average pore size of 1.45 nm. Presence of porphyrin ring helps for high redox activity and high accessible micropores helps for facile ion storage inside the COF matrix. From the electrochemical study, it was observed that the PT-COF shows a specific capacitance of 1443 F g^{-1} at a current density of 1 A g^{-1} with 91% capacity retention after 3000 cycles (at 5 A g^{-1}). It is postulated that the porphyrin goes for two electron oxidation/reduction process in acidic medium (0.5 M H_2SO_4). Thus, the pseudocapacitance coupled with the EDLC enhance the capacitance significantly.

Design and Development of Efficient Electrocatalyst for Water Splitting

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Conventional generation of electricity using fossil fuel produce toxic gases creating serious environmental issues. Therefore, there is a need for generation of electricity by using a green process. The Hydrogen and oxygen production by water electrolysis in conjunction with electrocatalysts is proposed as a critical route to address the carbon footprint concerns. Therefore, in this study, an eco-friendly, affordable and expansible process was carried out for the synthesis of Co_3O_4 nanomaterials as electrocatalyst for oxygen evolution reaction (OER) using orange peel (OP) extract as reducing agent in presence of universal solvent (H_2O) by dipping/absorbing and calcining, simple two-steps method. Several techniques were used to characterize the Co_3O_4 nanoparticles calcined at different temperatures including XRD, FT-IR, FESEM, TEM, XPS and BET. To study the effect of temperature on OER activity, as-prepared Co_3O_4 was calcined at 250, 450 and 650 °C temperatures and notably the best result for OER electrochemical performance was found at 450 °C with an overpotential of 328 mV@10 mAcm^{-2} having Tafel slope of 101 mVdec^{-1} and a small charge transfer resistance (5.13 Ω). The as-prepared sample's good electrocatalytic OER property at the calcining temperature 450 °C (Co_3O_4 -450) is mainly ascribed to its unique morphology, immense surface area, unique pore size and, the perfect structural defect promoting efficient adsorption, activation, and fast electron transfer of the reactant molecules eventually promoting OER activity.

NiWO₄ /Reduced Graphene Oxide Nanohybrid: An Efficient Bifunctional Electrocatalyst for Anodic Urea Oxidation and Cathodic Oxygen Reduction

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The efficiency of direct urea fuel cell (DUFC) mainly depends on the anodic urea oxidation reaction (UOR) and cathodic oxygen reduction reaction (ORR) kinetics. The design and development of efficient economic electrocatalysts for UOR and ORR remains a key for practical implementation of DUFC. Herein, we demonstrate a single step hydrothermal synthesis of NiWO₄ NPs/rGO composite for catalyse both UOR and ORR. The as synthesized NiWO₄ NPs/rGO composite catalyse UOR efficiently with a high oxidation current (212 mA/cm²) and exhibits less catalyst poisoning. Moreover, the NiWO₄ NPs/rGO composite shows a quasi 4 electron ($n = 3.92$) reduction path for molecular oxygen electroreduction. Oxygen reduction performance of the present composite is found comparable to the state-of-the-art Pt/C catalyst. In addition, the bifunctional electrocatalytic behavior of the NiWO₄ NPs/rGO composite is found superior as compared to pristine NiWO₄ NPs, physical mixture of NiWO₄ NPs and rGO, mixture of NiO and WO₃, NiO and WO₃. The improved electrocatalytic efficiency of the NiWO₄ NPs/rGO composite originates from the synergetic physiochemical properties of NiWO₄ NPs and rGO which facilitates analytes diffusion, reduces charge transfer resistance, and offers a greater number of active sites for the catalytic reactions.

Carbon Based Materials for the Sustainability of the Perovskite Solar Cells Within Radiation Environment for Space Grade Solar Cells

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Triple-cation perovskite solar cells (PSCs) have demonstrated excellent efficiency and stability for terrestrial applications; however, their vulnerability to radiation-induced degradation limits their suitability for space-grade solar cells. In this work, we will show the stability of triple-cation PSCs containing iodide and bromide halides under varying doses of gamma radiation. Our results reveal that gamma radiation significantly deteriorates device performance, primarily through reductions in short-circuit current density, attributed to perovskite layer degradation and reduced transparency of ITO glass substrates. Electron microscopy and photoluminescence analyses indicate iodide irregularities and radiation-induced defects, leading to phase segregation within the perovskite structure, while bromide and nitrogen atoms remain comparatively stable. These findings underscore the critical challenge of radiation resilience for PSCs in space environments. To address this, we propose the incorporation of carbon-based materials—such as graphene, carbon nanotubes, and carbon quantum dots—within PSC architectures. Carbon materials offer exceptional radiation-shielding properties, high electrical conductivity, and chemical stability, which can mitigate defect formation and enhance charge transport under high-radiation conditions. Their integration into perovskite layers, charge transport interfaces, or encapsulation structures provides a sustainable pathway to improve durability and maintain efficiency in space-grade PSCs. This work not only highlights the detrimental effects of gamma radiation on PSCs but also introduces carbon-based strategies as a promising solution for developing radiation-resistant, sustainable perovskite solar cells for space applications and advanced radiation detectors.

Catalytic Enhancement on Hydrogen Generation from Lithium Aluminum Hydride via Thermolysis

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Considering the current alarming trends in environmental contamination and fossil fuel depletion. In the search for renewable and clean energy sources, hydrogen is emerging as a possible alternative fuel, with current research concentrating on its storage and performance under optimal conditions to serve both mobile and stationary applications. As a result, sodium borohydride (LiAlH_4) is regarded as a potential hydrogen storage material (10.6 wt%) capable of producing hydrogen at low temperatures with rapid kinetics. Therefore, the effect of temperature needs to be investigated, and the optimal temperature for maximum hydrogen generation from sodium borohydride is crucial to characterize the material. The dry ball milling method was used to prepare the composite material (catalyst/ LiAlH_4). The synthesized materials were tested at various temperatures (75 °C to 300 °C) for hydrogen generation by thermolysis. X-ray diffraction, TG-DTA, Raman spectroscopy, and Fourier Transform Infrared spectroscopy are used to characterize the properties of the materials developed. The ideal conditions were 100 °C at atmospheric pressure. Lithium aluminum hydride decomposition was improved after 30 min at 100 °C, with catalyst additions. the composite material generates hydrogen 10(Catalyst)/ LiAlH_4 (1.81% wt%) > Pure LiAlH_4 (0.72% wt%). The hydrogen generation gradually increased with the thermolysis temperature.

A Study on the Influence of Biowaste and Energetic Ions on the Piezoelectric Phase & Energy Harvesting from Polymer Composite Films

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In the present study, a piezoelectric polymer-biowaste composite of poly(vinylidene fluoride) (PVDF) and biowaste rice husk (RH) has been reported. The hybrid displays a high piezoelectric b phase of 85% at the lowest RH concentration compared to the pure PVDF film with 74% b phase. However, as the RH concentration increases, the b phase, along with the mechanical strength, is witnessed to decrease. To overcome this short-coming, 2-D molybdenum disulfide (MoS_2) filler was added into the polymer matrix. The mechanical strength as well as the b phase was then found to increase. Further, low energy He^+ ion irradiation is performed on the films, which increases the b phase of the films. Preliminary energy harvesting experiments are carried out with a constant force and under regular day-to-day activities like finger tapping, bending and heel-pressing. Output voltages of $\sim 2\text{V}$ and $\sim 10\text{V}$ have been obtained under constant force and finger tapping. These results will be discussed in detail at the conference.

Turning Paper into Power: Sustainable Separator Innovation for Lithium-Ion Batteries

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Battery separators must electrically isolate electrodes while enabling ion transport, requiring porosity, wettability, mechanical/thermal stability, safety, and sustainability. Commercial separators are dominated by polyolefin-based separators, primarily polypropylene (PP) and polyethylene (PE), but their poor wettability, thermal instability, and environmental concerns limit performance. Alternatives such as modified polyolefins, synthetic polymers (PET, PAN, PVDF), and cellulose-based materials have been explored, with cellulose offering renewability, low cost, and strong electrolyte affinity. Here, cellulosic paper was functionalized with ceramics to create advanced separators. The ceramic-impregnated paper separator (PAPERATOR) exhibited excellent wettability (216-270%), quicker electrolyte saturation, improved mechanical strength (43.96-50.15 MPa), and thermal stability (no shrinkage up to 200 °C). The electrochemical cell comprising Graphite|PAPERATOR|LiFePO₄ cell delivered comparable performance to commercial PP/PE separators in terms of capacity retention at different current densities (0.05-0.8 mA cm⁻²), with stable cycling (300 cycles), high coulombic efficiency (>96%), and robust rate capability. Similarly, an LLZO-loaded paper separator (PAPELYTE) achieved high ionic conductivity (1.23 mS cm⁻¹), superior Li⁺ transport (t_{Li^+} = 0.64), and a wide electrochemical window (> 5.5 V). These breakthroughs enable the concept of electroactive paper separators for flexible paper-based cells, paving the way for future electronics such as wearable devices, foldable displays, and smart textiles.

A Reliability Engineering Perspective on Conventional Fuel Systems

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Conventional fuels, including coal, petroleum, and natural gas, remain a vital part of the world's energy supply. However, their dependability is now under risk due to a range of issues such as the exhaustion of resources, unstable supply networks, inconsistent fuel quality, and environmental limits. This study examines the reliability of conventional fuel systems by looking at the factors that affect steady energy generation, efficient operations, and long-term viability. Based on reliability engineering methods, the research investigates potential failures that occur during fuel extraction, refining, delivery, and storage, as well as issues related to the performance of combustion systems in power stations and industrial settings. The study also shows how aging infrastructure, political instability, and environmental regulations add to the risks of fuel supply and energy stability. The results stress the importance of better monitoring, proactive maintenance strategies, and diversified energy strategies to maintain the dependable functioning of systems that rely on conventional fuels.

Keywords: Conventional fuels; Combustion system performance; Reliability engineering; Resource depletion; Predictive maintenance.

An Optimized Matrix Scheme for Photovoltaic Array Under Partial Shading to Obtain Enhanced Power Generation and Profits

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A new reconfigured photovoltaic array (PVA) topology is proposed using a new technique namely Optimized Matrix Scheme (OMS). This novel topology is most efficient in reducing the line losses due to elongated conductor paths and lowering the unfavorable impacts of inconsistent partial shading (PS) ensuring unvarying distribution of the PS impacts on the PVA. The simulations are performed using MATLAB/Simulink to estimate the performance of OMS reconfigured technique in the influence of seven distinct insulations, including top left block PS, top right block PS, bottom left block PS, bottom right block PS, center block PS, oblique edge PS, and dual corner PS. The analysis for the PVA performance under the OMS technique is carried out for various parameters such as power imbalance ratio, efficiency index, fill factor, mismatch power loss, line loss index, global maximum power point, yearly stability factor and percentage of energy enhancement per day. The results show that the OMS topology produces 30.989 kWh of energy per day, surpassing the four schemes total cross tied, non-symmetrical puzzle pattern, ken-ken puzzle pattern, and matrix square PVA configuration. The annual revenue generated by a $[9 \times 9]$ OMS topology is estimated to generate an annual income of ₹ 151,0032.44, which is higher than all the four schemes considered for this study. In addition, the superiority of the proposed technique is proved by the reduction in the line loss upto 35.16%. Mismatch losses are also diminished by 773.1 W, which ensures a more stable and uniform generation of power across the PVA. Overall, the OMS topology exhibits significant improvements in electrical performance, energy efficiency, lowering line losses, and economic viability, thus making it an effective and sustainable solution for the PVA.

Novel Puzzle Pattern to Augment the Performance of Solar Photovoltaic Arrays Operating Under Partial Shading Conditions with Experimental Validation

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The performance of solar photovoltaic (PV) systems is notably hampered by partial shade, which can reduce the output power and efficiency significantly. Extensive research has been conducted to address this issue by minimizing partial shading (PS) effects in PV arrays (PVAs) through multiple configurations and reconfiguration techniques. This paper conceptualizes novel solar PVA topologies (PVATs) aimed at refining the power output generated by PVA working in conditions of PSs. Through a rigorous examination of six shading patterns applied to seven different array configurations, this study introduces five new PVATs, developed to minimize the partial shading effects on PVA. The study incorporates a 16-panel, 4×4 , 4 kW solar PVA, with each panel rated at 250 W. The performance of these newly proposed PVATs was assessed using MATLAB/Simulink simulations, after which a comparative analysis was done for testing their effectiveness with that of conventional array models under various PS conditions (PSCs). The results of this comparison highlight the superior performance of the modified total cross-tied (TCT) configuration, which, in certain PSC scenarios (especially top narrow and central wide) achieved upto 99% increase in output power compared to the standard TCT configuration. The practical applicability of the proposed method was further validated through experimental tests on the proposed 9×9 TCT PVATs. This research provides critical insights for PV power plant installers regarding the selection of prime scheme for array configurations, thus facilitating the enhanced utilization of solar energy resources.

Development of Supercapacitor Electrode Material Using Heavy Metal Adsorbed Buffalo Bone Char–Prosopis Juliflora Composite

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This project integrates waste valorization and energy applications. First activated carbon is created from bio waste and eco-invasive plant - Prosopis Juliflora. The activated carbon composite is used to treat simulated waste water with 4 different heavy metals (Cr, Zn, Cu, Fe). The used adsorbent is tested as a sustainable supercapacitor electrode material. After the thermal and chemical activation, its surface morphology and functional groups were identified using FTIR and FE-SEM analyses. The simulated waste water is treated under 3 different pH, 3 ratio of bone and wood char, and 3 different absorbent dosage. We have used Response Surface Methodology (RSM) was used to optimize the experimental parameters affecting adsorption and find the most optimized condition. The produced activated carbon was well-suited for electrochemical use due to its highly functional surface and well- developed porous structure. Excellent capacitive behavior with good stability and conductivity was confirmed by electrochemical evaluations using Galvanostatic Charge– Discharge (GCD), Electrochemical Impedance Spectroscopy (EIS), and Cyclic Voltammetry (CV). The findings show that the Prosopis Juliflora–regenerated bone char composite is a viable, affordable, and environmentally friendly material for good-performance supercapacitor electrodes. This work offers a circular strategy that connects renewable energy storage and wastewater treatment, encouraging environmentally friendly resource use.

Global Wind Energy Potential Assessment and Forecast on an Effect of Paris Agreement

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The fast depletion of fossil fuels and global warming made us to move towards the utilization of renewable energy, and most permissible sources are solar, wind, hydro and Bio energy. Paris Climatic agreement has provided the road map for renewable energy initiatives among the 195 countries. Each participants articulated their National Determined Contribution (NDC) with the amicable target year of 2030. In this paper investigate the possibility of attaining the mid-level targets based on the NDC definitions through wind by the Major economic countries in the world. To install the wind turbines, parameters like average wind speed, wind density and Weibull parameters are indispensable to estimate the amount of energy production, Levelized Cost of Energy (LCOE), and Energy Return on Investment (EROI). Small wind turbines and their purpose to society have been investigated and articulated. As per the current situation, explored sites could manage to contribute towards NDC for some of the countries, other countries need to explorer in vigour manner. Offshore wind energy has higher potential, and it has not yet been utilised to its full potential in many countries.

Thermal Instability Analysis for Enhanced Heat Transfer in Geothermal Porous Reservoirs

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Efficient extraction of geothermal energy strongly depends on convective heat transport mechanisms occurring within subsurface porous reservoirs. Understanding the onset of thermal instability in such systems is crucial for maximizing heat recovery while ensuring long-term sustainability. In this study, a comprehensive stability analysis of buoyancy-driven convection in saturated geothermal porous media is presented. The porous matrix is modeled using Darcy's law along with the Boussinesq approximation, incorporating realistic thermal boundary conditions representative of geothermal operations. The effects of permeability, Rayleigh number, reservoir depth, and thermal dispersion on the critical conditions for instability are systematically investigated. Linear stability theory, supported by numerical eigenvalue computations, is employed to predict the transition from conduction-dominated to convective heat transfer regimes. The results reveal that both spatial variation in permeability and enhanced thermal dispersion promote earlier onset of convection, enabling improved heat extraction. The findings provide valuable insights for optimizing reservoir design and operating parameters to improve thermal performance of geothermal systems. This analysis contributes to advancing energy-efficient utilization of geothermal porous formations, supporting the broader goals of sustainable and low-carbon energy technologies.

Keywords: Geothermal energy; Porous media; Thermal instability; Heat transfer enhancement.

CO₂ Activation on Pristine and Defected 2D Fe₂O₃ Monolayer: A First-Principles Study

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The adsorption and activation of CO₂ on two-dimensional transition metal oxides hold promise for advancing carbon capture and utilization (CCU). In this work, we employ first-principles density functional theory (DFT) to investigate CO₂ interaction with pristine and defect-engineered Fe₂O₃ monolayers. Pristine Fe₂O₃ exhibits chemisorption of CO₂ with an adsorption energy of -1.09 eV, accompanied by substantial molecular bending ($\angle\text{O}-\text{C}-\text{O} \approx 128-129^\circ$). Introduction of oxygen (V_O), iron (V_{Fe}), and combined oxygen and iron (V_{FeO}) vacancies further enhance binding strength (-1.27 to -2.31 eV) and modifies activation pathways. Notably, Fe vacancies exhibit the strongest adsorption capacity, whereas oxygen vacancies most effectively activate CO₂ through geometric distortion and vibrational softening, as evidenced by pronounced redshifts in symmetric and asymmetric stretching modes. In contrast, Fe-related vacancies stabilize a nearly linear CO₂ geometry ($\angle\text{O}-\text{C}-\text{O} \approx 176-179^\circ$) with weaker activation despite strong adsorption. These findings highlight a dual role of defects: oxygen vacancies optimize molecular activation, while Fe vacancies maximize adsorption strength. This work establishes a clear structure and property relationship and provides design principles for defect-engineered Fe₂O₃ monolayers as efficient 2D catalysts for CO₂ conversion in sustainable energy and chemical applications.

Green Chemistry on the Runway- Sustainable Fashion Hues from Agro-Waste

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Chemistry has always been an integral part of the fashion industry, influencing fiber development, textile finishing, processing and color creation etc. In recent years, sustainability has become a central concern, driving the adoption of eco-friendly practices in production and textile processing. One promising approach involves the use of natural dyes derived from fruits, vegetables, and other plant-based agro-waste, including pomegranate peels (tannins, ellagic acid), onion skins (quercetin), turmeric rhizomes (curcumin), marigold petals (lutein, carotenoids), hibiscus flowers (anthocyanin) etc. These bioactive compounds provide renewable, cost-effective, and environmentally benign sources of textile coloration. Application on natural fibers such as cotton, silk, and wool is enhanced by mordents, while green chemistry-based extraction ensures minimal chemical load on environment. Collaborative efforts between chemists and fashion practitioners enable the translation of these natural compounds into practical, durable, and commercially viable textiles. This approach exemplifies a “waste-to-wardrobe” model, opening avenues for entrepreneurial ventures, startups, and research innovation. In the present paper, we review and compile information on various agro-waste-derived dyes, their chemical properties, extraction methods, and applications, providing a comprehensive resource that can guide researchers, designers, and industry stakeholders toward sustainable and innovative textile solutions.

Efficient Catalyst-Free Domino Process for Conjugate Addition and Decarboxylation of Coumarin Carboxylic Acids/Esters with Pyrazolones: A Green Chemistry Approach

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A methodology for tandem conjugate addition, decarboxylation, and esterification/amidation of coumarin 3-carboxylic acid derivatives with Pyrazolones has been developed. The reactions were conducted using coumarin 3-carboxylic acid or its esters and Pyrazolones in an alcohol solvent, resulting in the formation of the corresponding pyrazolyl 2-hydroxyphenylpropionate derivatives. For the amidation process in the addition reaction, amines and environmentally friendly solvents were utilized. This approach offers numerous advantages, including excellent yields, a broad substrate scope, operation without catalysts, straight forward purification through simple filtration without any extensive workup, mild reaction conditions, and the elimination of organic solvents, ligands, bases, and additives. This green and versatile synthetic protocol is applicable to the synthesis of substituted pyrazolyl phenyl propionate and amide derivatives. Furthermore, this method emphasizes the importance of the coumarin 3-carboxylic acid/ester core structure in the Michael addition process.

IoT-Enabled Multi-Parameter Monitoring System for Real-Time Snow Avalanche Disaster Management

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Monitoring and forecasting avalanches are important for safety purposes and can be achieved using real-time data monitoring. Realistic snow avalanche risk assessment requires continuous monitoring of key environmental parameters under harsh high- altitude conditions. This work presents a solar-powered, IoT-enabled avalanche monitoring system designed to acquire and process multiple environmental parameters, including wind speed, wind direction, ambient temperature and humidity, and snow depth. The system incorporates a high-resolution 24-bit data acquisition module with local storage, ensuring accurate measurements and secure data logging. Data are transmitted via a low-power, long-range wireless (LoRa) link to a receiver unit, which forwards the information to a cloud server through an API for real-time visualization and analysis. The design has been validated for operation at temperatures as low as -25 °C, with reliable data transfer demonstrated over a 5 km line-of-sight range in mountainous terrain. The proposed framework provides a scalable, energy-efficient, and cost-effective solution for avalanche parameter monitoring, with broader applications in disaster management, climate studies, and renewable energy resource assessment. The real-time monitored data can be used for forecasting using a pattern recognition technique with historical data.

Decoding Photo-Catalytic Degradation using Spectral Data Fusion via Multivariate Curve Resolution and Bayesian Modelling of Industrial Wastewater

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The photocatalytic remediation process presents specific challenges due to the complex nature of the molecular degradation process and the lack of intermediate information. Combined Advanced oxidation process (AOP)- based wastewater treatment techniques result in complete dye remediation (>98%), paving the way for pilot-scale industrial deployment. The photocatalytic degradation of industrial reactive dyes is monitored simultaneously using spectroscopy and chromatography techniques to characterize, identify, and resolve the intermediate compounds of the degradation products. This work employs a workflow for degradation analysis that combines spectral and chromatographic data to elucidate the degradation mechanism, utilizing chemometric analysis and statistical inference techniques for industrial dye wastewater. Bayesian inferential modelling and multivariate curve resolution techniques, utilizing mid-level data fusion, facilitate the retrieval of intermediate sample concentration and spectral estimation profiles, thereby deriving quantified reaction rates for the solar-induced hydroxyl attack mechanism on industrial dyes. This helps in accurately identifying and predicting outcomes in the presence of uncertainties and establishes a quantitative framework for the molecular decay of the dyes and remediation of the degraded samples.

Hydrochemical Study and Heavy Metal Pollution Analysis of the Chhoiya River

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The present study focuses on the hydrochemical characteristics and analyzes the pollution status of the Chhoiya River, caused by heavy metal. The Chhoiya River is a crucial source of water in the Bijnor district, U.P., region. Rapid urbanization in the areas surrounding the river has contributed to the spread of several serious health problems, including cancer, skin disorders, cardiovascular disease, and even premature death. So there is a need to evaluate the water quality of the river. Physico-chemical parameters such as pH, electrical conductivity, total dissolved solids, hardness, alkalinity, acidity, dissolved oxygen, biological oxygen demand, chemical oxygen demand, and turbidity were systematically analyzed. Additionally, the concentration of noxious heavy metals (such as arsenic, cadmium, chromium, nickel, and lead) was evaluated using standard analytical techniques (ICP-MS). We collected samples of water from different locations at intervals of three months' duration (summer, monsoon, and winter). We assessed the overall water quality using the water quality index (WQI) and heavy metal pollution index (HPI). The analysis of physicochemical parameters and heavy metal concentration revealed distinct spatial and seasonal variations. The result showed the influence of natural processes and anthropogenic activities, including agricultural runoff, urban wastewater discharge, and industrial effluents. The level of heavy metal concentration exceeded permissible limits of WHO and other national standards. In all seasons, the water quality index, along with physico-chemical parameters and heavy metal concentration, exceeded the permissible limits, indicating a highly deteriorated water quality status. An elevated level of heavy metal is a potential risk to aquatic organisms and local communities dependent on the river water for different purposes. The Chhoiya River suffers from a serious threat of industrial pollutants, which may increase the life threat of heavy metals such as arsenic and lead. So, this study highlights and focuses on the immediate requirement for continuous monitoring, effective management methods, reducing the discharging of waste effluents from industries, and pollution mitigation measures to safeguard the ecosystem health of the Chhoiya River and preserve the long-term availability of its water resources.

Keywords: Hydrochemistry; Water Quality Index (WQI); Heavy Metal Pollution Index (HPI); Anthropogenic impact; Seasonal Variation

Assessment of River Water Quality Using Water Quality Index (WQI) Method

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Rivers are the highly responsive freshwater habitat that plays a important role in supporting human settlement, agriculture productivity, and aquatic biodiversity. However, accelerated industrial growth, expansion of urban areas, and agricultural intensification, which is leading to notifying significant degradation of river water purity in many areas of India. The present study focuses on the evaluation of river water purity by using the Water Quality Index (WQI) method, which provides a single numerical data which representing the overall quality of water for various purposes. To evaluate seasonal fluctuations, water samples were collected from different sites along the river during pre-monsoon, monsoon, and post-monsoon seasons. Physico-chemical parameters of river water for evaluating the water quality index including pH, conductivity, total dissolved solids, hardness, alkalinity, dissolved oxygen, biochemical oxygen demand, chemical oxygen demand, chloride, nitrate, sulphate, and heavy metals such as lead, cadmium, nickel, arsenic and chromium were analyzed following standard methods suggested by APHA.

The obtained data were statistically processed and compared with the permissible limits set by WHO and BIS guidelines. The WQI values were calculated to classify water purity into different categories such as excellent, good, poor, very poor, and unsuitable for different purposes such as drinking. The obtained data shows the fluctuations in seasonal variations in water quality, with deterioration in water quality during the pre-monsoon period due to decreased dilution and increased pollutant amount. Those sampling sites located near the areas of urban settlements and industrial effluent discharge points exhibited higher WQI values, indicating severe anthropogenic activities. The overall obtaining results suggest that the river water in the studied region requires more focuses, proper management, periodic monitoring, and implementation of sustainable pollution control strategies. This study highlights the usefulness of WQI as an effective tool for evaluating surface water quality and supporting environmental management policies.

Sunlight-Driven Photocatalytic Degradation of Methylene Blue Using NiO/rGO Nanocomposites

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Rapid urbanization and industrial growth have resulted in the discharge of various pollutants into aquatic systems, posing serious environmental and health concerns. Among these pollutants, organic dyes from textile, paint, and pigment industries are highly toxic, chemically stable, and resistant to degradation. Their persistence not only alters water quality but also impedes light penetration, adversely affecting aquatic ecosystems. Photocatalysis has emerged as an efficient and economical technique for the degradation of such pollutants, as it transforms toxic organic compounds into less harmful fragments without generating secondary contaminants. In this study, NiO/rGO nanocomposites were synthesized via a hydrothermal method followed by calcination and utilized for the photocatalytic degradation of methylene blue dye. The prepared nanocomposites were characterized using X-ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), Raman Spectroscopy, and Fourier Transform Infrared Spectroscopy (FTIR), while surface area was determined using the BET surface area analyzer. Photocatalytic experiments indicated that NiO/rGO exhibited significantly enhanced degradation performance under sunlight compared to dark conditions, achieving a remarkable 99% removal of methylene blue within 30 minutes. The effects of catalyst dosage, pH, and contact time on degradation efficiency were also investigated. The findings suggest that NiO/rGO nanocomposites possess excellent photocatalytic activity and hold strong potential for the rapid and effective removal of organic dyes from wastewater.

Development of an Ambient Air Quality Index for the Assessment of Pollutants and Heavy Metals Using Fuzzy Logic

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Urban and industrial regions constantly face increasingly complex air pollution challenges. Policy makers rely heavily on-air quality indices to make regular assessments of quality and prioritize remediation strategies. Although conventional air quality indices exist to give a measure of the overall quality, they are unable to do justice to uncertainty and nonlinear interactions among parameters. This study presents the development of a Fuzzy Logic-based Ambient Air Quality Index to evaluate the cumulative impact of criteria air pollutants and eight heavy metals in ambient air. The fuzzy inference system integrates linguistic variables and expert-defined membership functions to translate complex, imprecise data into a single, interpretable air quality index. Employing a Mamdani-type fuzzy inference system, Linguistic rules and membership functions were formulated through expert judgment and validated using measured air quality data from representative urban monitoring stations. The proposed index provides smoother gradations of air quality classes and enhanced sensitivity to heavy-metal concentrations compared with traditional AQI approaches. The proposed fuzzy-based index thus offers an adaptable and intelligent framework for decision-makers to evaluate ambient air quality and prioritize action.

Keywords: Air quality; AQI; fuzzy logic AQI; limitation of existing AQI

Screening and Characterization of Inhibitory Action of Phytoproducts Against *Candida Albicans* an Opportunistic Fungal Pathogen

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The name *Candida* was proposed by Berkhout. *Candida albicans* is a dimorphic and ubiquitous fungus that exists in warm-blooded animals as a naturally occurring organism in the intestinal tract or microbiome of the human body and propagates via blastospore phenotype (also called blastoconidia). Blastospores are characterized by their oval shapes, mononucleated cells and propagation through cellular budding. *Candida albicans* is able to transform into one of two filamentous forms: pseudohyphae and hyphae. *Candida* is thin-walled, small yeast (4 to 6 microns) and innocuous in most individuals, but under certain circumstances, they can opportunistically overgrow and cause disease. *Candida albicans* resides as commensal or endosymbionts in the oral cavity, skin, digestive tract and genital region of healthy individuals. While it also causes superficial infections and life-threatening systemic mycosis in the immuno-compromised individuals like- HIV infected patients, organ transplant patients, chemotherapeutic patients and those with indwelling devices [2]. *Candida albicans* causes chronic infections of the skin and nails and also found in the environment particularly on leaves, flowers, water, and soil. Almost 75% of women at childbearing age suffer from vulvovaginal (VVC) candidiasis and 45% of these women have at least one recurrent infection. Candidiasis is non-discriminate and men can be infected as well. *C. albicans* now ranks as the fourth leading cause of nosocomial infections and the most common fungal species present in bloodstream infections, with mortality rate of 38% to 49%. Candidiasis is becoming a serious public health problem in the past several decades with increasing incidence of multi drug resistance (MDR), emerging drug resistant strains and failure of therapy. Therefore, this paves way to develop new therapeutic strategy to combat MDR.

Enhancing CO₂ Capture: Composite Ionogel Membranes with DES-IL Blends for Efficient Gas Separation

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The increasing levels of carbon dioxide (CO₂) have highlighted the urgent need for effective strategies to mitigate global warming. Deep eutectic solvents (DES), considered a promising alternative to ionic liquids, have recently gained attention as a novel class of environmentally friendly solvents with potential applications in gas separation. To enhance the efficiency and cost-effectiveness of CO₂ capture technology, a composite ionogel membrane is developed using DES and IL blend and a polymer. Here Pebax 1657 used as a selective layer for CO₂ separation from CO₂/CH₄ mixture, with PVDF as a support. Novel blend consisting of Choline Chloride and Ethylene Glycol DES with [THTDP][Cl] IL is then used as an additive to enhance the CO₂ permeability. The synthesized blend has been characterized using FTIR Spectra. Different concentration of blend has been added to check the effectiveness of membrane performance. Fabricated membranes were characterized using FTIR, XRD and SEM. Permeabilities of both pure and mixed gases have been calculated. Prepared membrane exhibits excellent permeability and selectivity compared to other DES -supported membranes. Density Functional Theory (DFT) study also used to optimise and analyse the interaction between IL and DES and further their interaction with both CO₂ and CH₄. This study shows that DES can be taken as a promising alternative for conventional amine solvents.

Keywords: Deep Eutectic Solvents, CO₂ Separation, Membrane Separation, Density Functional Theory, Ionogel Membranes.

Probabilistic Accident Risk Assessment of the Railway System Using A Fuzzy Bayesian Network: An Indian Case Study

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Indian Railways network is the fourth longest in the world, but in the past few years, railway accidents have been on the increase in India. In the last 30 years, around 170 railway accidents were reported, causing around 3500 fatalities and 6500 injuries and more environmental damage. This necessitates the need to conduct an elaborate risk assessment of the railway infrastructure system. Though few studies were performed on railways around the world, an elaborate quantitative safety risk assessment in the field of railways has not been studied thoroughly. In this work, a Fish Bone diagram is constructed with the help of expert inputs to find the causes of the railway accidents, and then fuzzy-based Bayesian network analysis is used to assess the risk of railway operations. Due to the availability of limited data, the presence of multiple causative factors, and to handle the uncertainty, a fuzzy system is used to convert the inputs of the various experts to Fuzzy probability values. Bayesian Network is utilized to represent causal and probabilistic dependencies between dominant risk factors and to estimate the prior risk probability risk value. Various factors like Environmental factors, mechanical failure, human factors, Management factors, sabotage, climatic factors were incorporated in the Fuzzy BN system. This work can be used to assess the existing risk of the railway system and also provides the means to understand the strong and weak factors to prevent the accident in railway system in the process of building sustainable infrastructure of India.

Production of Fuel Additives through Glycerol Acetylation over Sulfated Metal Oxides

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Acetylation of glycerol signifies a promising route for the valorization of glycerol, a major by-product of biodiesel production, into value-added chemicals such as monoacetin, diacetin, and triacetin. These acetins are widely used as bio-additives, plasticizers, and solvents due to their favorable physicochemical properties. In this study, the acetylation reaction was carried out using acetic acid as the acetylating agent in the presence of various solid acid catalysts, including zirconium oxide (ZrO_2), tungsten oxide (WO_3), sulfated zirconium oxide ($\text{ZrO}_2\text{-SO}_4^{2-}$), sulfated tungsten oxide ($\text{WO}_3\text{-SO}_4^{2-}$), and sulfated mixed oxide catalyst ($\text{ZrO}_2\text{-WO}_3/\text{SO}_4^{2-}$). The catalysts were synthesized via thermal decomposition and wet impregnation methods, and characterized using XRD, SEM, and FTIR to evaluate their structural, morphological, and chemical properties. The sulfonated catalysts exhibited enhanced Brønsted acidity, leading to higher conversion of glycerol and greater selectivity toward triacetin. Parametric studies were performed for change in time, temperature, catalyst loading and mole ratio. Under optimum condition of 120°C , molar ratio of 1:6 and 1.0% catalyst loading $\text{ZrO}_2\text{-WO}_3/\text{SO}_4^{2-}$ gave the highest conversion of 95.3% with 24.4% selectivity to triacetin in 9h of reaction time.

Keywords: Glycerol acetylation, Sulfated metal oxides, Triacetin, Diacetin, Monoacetin

Reliability and Availability Analysis of Polymeric Materials Under Environmental and Mechanical Stressors

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Polymeric materials are commonly used in structures, electronics, and industries because they are light, flexible, and affordable. However, their performance and how long they last are greatly affected by environmental factors like temperature changes, sunlight, moisture, chemical contact, and physical wear. This research introduces a method to evaluate the reliability and availability of these materials by looking at how they break down over time. The analysis uses probability-based models to show how materials degrade, considering time-related changes, aging processes, and different ways they can fail, such as cracking, becoming brittle, slow deformation, and layers separating. Key reliability measures like average time until failure, chances of failure, and availability are calculated by combining real-world aging data with statistical models. The findings show how environmental conditions speed up material breakdown and lower their usefulness, emphasizing the need for reliable predictions in designing, choosing materials, and managing their use over time. The framework helps in better predicting how polymers will perform and aids in creating stronger, more suitable polymer-based systems for specific uses.

Keywords: Polymeric materials; Reliability analysis; Availability assessment; Material degradation; Ageing kinetics; Environmental stressors.

Integrating Solid Waste Management into Urban Sustainability in Uttarakhand: A Detailed Analysis of Legacy Waste Management and Dump Site Remediation with SDG Benchmarks

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The principles of sustainability for growing cities are essential for balance between environment and development. These principles are driven by United Nations sustainable development goals (SDGs) SDG11: Sustainable cities and communities and SDG 13: Climate Action. In line with this, the state government of Uttarakhand, India is aiming for effective solid waste management (SWM) in Dehradun and other cities to meet urban sustainability and SDGs. The state authorities are working hard on 'legacy waste management and dump site remediation' in SWM and committed to remediate those sites as per CPCB guidelines for Legacy Waste Biomining, 29.04.2019 and 'Swachh Bharat Mission (SBM)' 2.0 toolkits. At present in the state, 14 detailed project reports of 13 Urban Local Bodies (ULBs) have been approved by Ministry of Housing and Urban Affairs (MoHUA), Government of India. These ULBs are responsible for effective solid Waste Management in all respects. Total 23 out of 61 legacy sites and around 10.5 lakhs out of 23 lakhs metric tons of legacy wastes were already remediated and 141.89 acres of land are targeted to make free. The work progress is satisfactory and the state's initiative is well appreciated at various platforms for achieving the SDGs.

Keywords: SDG, Sustainability, Legacy waste, Urban local bodies

Microbial Contamination and Water Quality Assessment of Surface Water in the Upper Indian Himalayan Region: Implications for Environmental Sustainability

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The upper Indian Himalayan region is characterized by its fragile ecosystems and dependence on surface water sources for drinking, irrigation, and tourism activities. However, increasing anthropogenic pressure, tourism, and climatic variations have heightened the risk of microbial contamination, posing a serious threat to environmental and public health. In the present study, surface water samples were collected from multiple Himalayan sites and analyzed for key physicochemical parameters (pH, turbidity, TDS, and temperature) and microbial indicators, including *Escherichia coli*, *Pseudomonas*, and total coliforms. The obtained data revealed significant spatial variations in microbial load correlated with human interference and environmental conditions. These findings highlight the urgent need for sustainable water management practices and periodic monitoring of microbial contamination in ecologically sensitive mountain zones. The study underscores the integration of microbiological surveillance with environmental sustainability strategies to ensure the long-term safety and conservation of Himalayan freshwater resources.

Keywords: Surface water, Microbial contamination, Water quality, environmental sustainability.

Real-Time Evaluation of Grid-Connected Solar PV System Using PVsyst

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The growing demand for renewable energy has made grid-connected solar photovoltaic (PV) systems a vital solution for sustainable power generation. Present study focuses on the real-time performance evaluation of a 100kWp rooftop PV system installed at Noida Institute of Engineering and Technology, Greater Noida, India. Using PVsyst software, the system was simulated to predict energy yield, performance ratio, and losses under site-specific conditions. Real-time operational data were collected and compared with simulated results to identify deviations and loss factors such as temperature, dust, and inverter inefficiency. The analysis revealed an annual energy production of 145.33MWh with a performance ratio of 82.58%, indicating efficient system operation. Findings emphasize the importance of integrating real-time monitoring with simulation tools for accurate performance assessment and optimization of grid-connected PV systems.

Techno-Economic Assessment and Simulation of Solar Water Pumping System

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The research investigates the technical and economic viability of solar water pumps using PVsyst simulation. The system contains a 5kWp PV array optimized at a 24° tilt angle, delivering an annual energy yield of 14.3MWh. The simulation results report a performance ratio of 78%, with losses primarily due to temperature (8%) and soiling (3%). The pump delivers 300–350 m³/day, meeting irrigation requirements efficiently. Economic analysis reveals a levelized cost of energy (LCOE) of ₹3.2/kWh, significantly lower than diesel alternatives. The system achieves zero operational emissions, avoiding 12–13 tons of CO₂ annually. Findings demonstrate that solar water pumping systems offer substantial cost savings, high reliability, and strong environmental benefits, making them ideal for rural and agricultural sectors.

Poster Presentations

Electrochemical Analysis of as Synthesized MnO₂, NrGO, NrGO-MnO₂ 2D Nanosheets for CO₂ Reduction

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The electrochemical reduction of CO₂ into value-added chemicals and fuels represents a sustainable pathway to mitigate greenhouse gas emissions while addressing the global energy challenge. In this study, nitrogen-doped reduced graphene oxide (NrGO), manganese dioxide (MnO₂), and a composite (NrGO-MnO) were synthesized and systematically characterized to investigate their potential as CO₂ reduction electrocatalysts. Structural and morphological analyses confirmed the formation of poorly crystalline MnO fragments uniformly dispersed on the NrGO framework, effectively preventing graphene restacking and enhancing surface accessibility. BET surface area analysis revealed that NrGO-MnO exhibited a significantly higher specific surface area and pore volume compared to pristine materials, while TGA and XPS confirmed improved thermal stability, nitrogen functionalities, and Mn-O electronic interactions within the composite. The electrochemical reduction of CO₂ (CO₂RR) into value-added products represents a promising route for carbon utilization and sustainable energy conversion. We evaluated the CO₂RR performance of MnO₂, NrGO, and their composite (NrGO-MnO) using a two-chamber, three-electrode setup. LSV confirmed catalytic activity for all, with NrGO-MnO showing the highest current density due to synergy between conductive NrGO and active MnO sites. EIS revealed its lowest charge transfer resistance, establishing NrGO-MnO as a promising electrocatalyst and underscoring the value of hybrid nanostructures in enhancing conductivity and activity.

Hot Deformation Behaviour and Constitutive Modelling of Al 6351 Alloy at Varying Strain Rate

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This work presents a comprehensive investigation into the high-temperature flow behaviour of a versatile aluminum alloy subjected to deformation at 200°C, 250°C, and 300°C under strain rates of 0.001 s⁻¹, 0.01 s⁻¹, and 0.1 s⁻¹. The experimental results provide essential insight into the alloy's thermomechanical response, enabling improved process design and extending its applicability in aerospace, automotive, and structural components. The understanding of thermomechanical behaviours enables the fabrication of nanostructured materials using deformation processes such as severe plastic deformation. To describe and predict flow stress evolution, two phenomenological constitutive models, the modified Johnson–Cook (m-JC) and modified Zerilli–Armstrong (m-ZA), were evaluated alongside an artificial neural network (ANN) framework. Furthermore, the kinetics of dynamic recrystallization (DRX) were quantified using the Johnson–Mehl–Avrami–Kolmogorov (JMAK) equation, providing insight into microstructural evolution during hot deformation. Comparative analysis revealed that while the m-JC model achieved reasonable accuracy with an average absolute relative error (AARE) of 4.20%, the m-ZA model demonstrated limited precision (AARE 11.56%). The ANN approach outperformed both models, achieving an AARE of 0.998%, underscoring its potential for capturing the complex interplay of nanoscale effects in flow behaviour prediction.

Keywords: Flow stress behavior, Nanostructure, Hot compression, flow stress prediction, DRX fraction.

Significance of Multi Axial Forging on the Anisotropic Properties of Al-Li 8090 Ultra-Fine-Grained Material at Various Processing Conditions

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In the current study, multi-axial forging was performed on the Al-Li 8090 alloy. Forged material goes through various successive passes for different conditions. The anisotropic properties of this material were extracted from uniaxial tensile test results. Three identical tensile specimens were formed, each with different processing conditions and also taken from the material at different orientation angles (0° , 45° , 90°). These properties were compared for the base, room temperature forged (cycle-6) and cryo forged (cycle-6) conditions of the material. Planar anisotropy (ΔR) and mechanical anisotropy (\bar{R}) are both significant factors that serve as benchmarks while evaluating the material's formability. The anisotropic properties were also discovered to be much better in the cryo forged cycle 6 condition as compared to other conditions.

Tailoring Pd₇Se₂ Nanoparticles via a Single Source Strategy for Efficient Hydrogen Evolution Reaction (HER)

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Development of nanosized materials has garnered attention in the last few decades due to their interesting properties such as stability, size, shape, recyclability and composition. In the present study, Pd₇Se₂ nanospheres have been synthesized via a simple and hassle-free route i.e., single source precursor method. In this method, a palladium complex (synthesized using a Se-donor ligand) is thermolyzed at 280 °C under N₂ atmosphere for 2 hours to obtain pure phase of Pd₇Se₂ NPs. The ligand and the palladium complex have been characterized using ¹H, ¹³C{¹H} NMR and IR spectroscopy. The Pd₇Se₂ NPs are also well characterized using FE-SEM, SEM-EDS, P-XRD, XPS and TGA. The nanoparticles are explored as electrocatalyst for HER. It requires an overpotential of only 162 mV to drive a current density of 10 mA cm⁻² and it also shows an extremely low Tafel slope value of 20 mVdec⁻¹. The electrocatalyst has also been characterized after performing HER studies using FE-SEM, SEM-EDS, P-XRD, and TGA.

Stable Gold Nano-Islands via Reactive Glass-Metal Interactions Under ambient Conditions

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Achieving stable gold nanoparticles with tunable surface compositions through reactive metal-support interactions (RMSIs) under ambient conditions remains a significant challenge. In this work, we present a novel approach—Reactive Glass-Metal Interaction (RGMI)—as an effective and sustainable strategy to fabricate gold nano-islands with enhanced thermal stability and tailored surface chemistry. By systematically tuning the composition of sodium aluminophosphosilicate (NAPS) glass, we demonstrate that glass chemistry directly governs interfacial behavior, allowing the formation of stable gold nanostructures at moderate temperatures (550 °C) in ambient air. This process bypasses the need for reducing agents, high-vacuum systems, or long reaction times—offering a scalable, environmentally friendly fabrication route. Na and P species from the glass intercalate at the gold interface, inducing Au(111) lattice distortion and forming new electronic states near the Fermi level. These features significantly improve hot carrier lifetimes, enhancing catalytic potential. RGMI offers a versatile route for engineering stable, functional nanostructures with applications in catalysis, sensing, and optoelectronics.

Rational Design of CsPbBr₃ @MOF Composites for Enhanced Photoluminescence and Sensing

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Metal-organic frameworks (MOFs) have emerged as versatile hosts for encapsulating halide perovskite, offering a promising route to enhance their structural stability and environmental tolerance. Among these, CsPbBr₃@MOF composites represent a unique hybrid platform combining the superior optoelectronic properties of all-inorganic perovskites with the tunable porosity and chemical functionality of MOFs. This work presents a comparative analysis of synthetic strategies reported for fabricating CsPbBr₃@MOF systems, like “Ship-in bottle, Bottle-around ship and One-pot synthesis” approaches within frameworks such as ZIF-8, MOF-5, Eu-BTC, and Cu-MOF. The choice of MOF topology, metal node, and linker functionality critically governs nanocrystal dispersion, quantum yield retention, and luminescence stability. Furthermore, these composites exhibit enhanced photoluminescence intensity and selectivity toward analytes such as volatile organic compounds, metal ions, and nitroaromatics, etc. highlighting their potential in sensing applications. This provides an integrated understanding of how interfacial interactions and confinement effects within MOFs can modulate the optical response of CsPbBr₃, paving the way for the rational design of perovskite@MOF hybrid sensors.

Bimetallic Ag-Au Nanoalloy Decorated Boron Nitride for High Performance Supercapacitors

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The need for advanced supercapacitors has been emphasised as a crucial step towards sustainable life and high-performance energy storage devices encouraged by portable electronics. Boron nitride offers exceptional thermal conductivity, remarkable dielectric properties and high mechanical strength but direct application in electronics is limited by its large band gap. To overcome this, silver-BN (Ag@BN) adds strong conductivity and a range of redox active oxides, gold-BN (Au@BN) contributes to exceptional stability and surface-plasmon resonance. In this study, fabrication and electrochemical assessment of nanoscale hybrid of Ag-Au nanoalloy synthesised via simple co-reduction procedure and decorated on boron nitride nanoparticles utilizing simple stirring method. The confirmation of nanocomposite formation was provided by characterisation techniques, UV-Visible spectroscopy, FTIR spectroscopy and Raman spectroscopy. The band gap value for BN was calculated to be 5.4 eV but facile integration of bimetallic nanoalloy in BN, culminates in lowering of band gap values to 5.0 eV, further enhancing electron transport and overall electrochemical performance. In this work capacitive characteristics, rate capability and cycling stability over repeated charge-discharge cycles of nanoalloy composite as compared to pristine boron nitride will be demonstrated.

Mechanical And Dielectric Properties of Porous Elastomer for Flexible Strain and Pressure Sensors

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Introducing porosity into dielectric elastomers offers an effective approach for tuning their electromechanical properties, thereby enhancing sensitivity, response time, and signal stability for flexible sensor applications. In this study, a porous PDMS elastomer is developed using sugar particles as a porogen and characterized for its mechanical and dielectric properties. Weight analysis and surface morphology confirmed successful pore formation. The mechanical behavior is examined on developed samples under tensile deformation up to failure and strain-controlled cyclic loading to realize the elasticity and durability, respectively. Also, the dielectric properties are characterized in terms of relative permittivity and dielectric loss over a wide frequency range to comprehend the effect of porosity on electrical energy storage capacity and dissipation behavior. Porosity in PDMS developed through sacrificial sugar particles is found to reduce the ultimate strength as well as failure strain, though these are reliable for strain/pressure sensing applications. Also, the porosity resulted in improved relative permittivity and reduced the dissipation factor as compared to solid PDMS. Porosity introduced into PDMS through a porogen is recognized as a promising strategy to tailor mechanical and dielectric properties, achieving a balance between flexibility, sensitivity, and energy efficiency, thereby advancing the design of high-performance flexible sensors.

Probing the Dielectric Landscape of KNN Thin Films with Surface Plasmon Resonance (SPR)

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Worldwide researchers are actively engaged in precise determination of dielectric constant and refractive index of insulating thin films in fields related to microelectronics, photonics and optical communication. Existing techniques including ellipsometry, interferometry and capacitance measurements involve complex setups, controlled environmental requirements or are dependent on error-prone model-based fitting. Surface Plasmon Resonance (SPR) is a robust technique known to utilize enhanced light-matter interactions, enabling sensitive determination of multi-component thin film characteristics. Literature reports identify Potassium Sodium Niobate (KNN) as a material of choice for photonics due to its strong electro-optic, nonlinear and piezoelectric properties, enabling efficient optical modulation.

In the current study optical and dielectric properties of potassium sodium niobate (KNN) based thin films have been investigated using SPR and UV-Visible (UV-Vis) spectroscopy techniques. Thin films of KNN synthesized at varying substrate temperatures have been deposited using RF magnetron sputtering, ensuring controlled stoichiometry and high-quality crystalline growth. Subsequently, evanescent wave has been excited using a thermally evaporated Au overlayer and SPR measurements carried out in Otto configuration. Observed variations in refractive index and dielectric constant helped gain a deeper insight about the domains of the films. UV-Vis studies have been utilized for the determination of optical transmittance, absorption and band gap characteristics.

Geotechnical Stabilization and Design Optimization of Overburden Dumps Using Fly Ash: Experimental and Numerical Approach

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The rapid expansion of opencast coal mining in India has led to the generation of substantial quantities of mine overburden (OB), while the concurrent rise in fly ash (FA) production from thermal power plants exacerbates environmental and disposal challenges. This study evaluates the geotechnical feasibility of utilizing FA as a stabilizing additive in OB dump formations through the development of engineered FA-OB composites. Comprehensive laboratory investigations including grain size analysis, Standard Proctor compaction, Direct Shear Tests (DST), and Unconfined Compressive Strength (UCS) tests were performed to assess material behaviour and mechanical performance. The results reveal that incorporating 30% FA achieves an optimal balance between shear strength and compressive resistance, beyond which particle bonding weakens and strength declines. Numerical simulations based on the Limit Equilibrium Method (LEM) were further employed to assess slope stability across varied dump geometries. An optimized configuration featuring a 2.5 m FA layer strategically placed in the lower to mid-bench region yielded a Factor of Safety (FOS) greater than 1.5, satisfying stability requirements. These findings demonstrate that FA-OB composites offer a sustainable and technically viable solution for enhancing slope stability while enabling beneficial reuse of industrial waste in large-scale mining operations.

Tuning Bismuth Stoichiometry to Suppress Secondary Phases in the Synthesis of BiFeO₃

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Bismuth ferrite (BiFeO₃) is a prominent multiferroic material which exhibits ferroelectric and antiferromagnetic properties at room temperature. However, the practical utility of this material is often hindered by the presence of secondary impurity phases such as Bi₂₅FeO₄₀, and Bi₂Fe₄O₉. In the present study, Bi-rich compositions of Bi_{1+x}FeO₃ ($x = 0.00, 0.01, 0.03, 0.05, 0.07$ and 0.1) were synthesized utilising sol-gel auto-combustion method with citric acid as chelating agent to systematically suppress the secondary phases. X-Ray Diffraction (XRD) with Rietveld refinement conveyed that a moderate Bi excess effectively minimizes the secondary phases to 4.1% and retains the rhombohedral perovskite structure. Scanning Electron Microscopy revealed spherical nanoparticles. X-Ray absorption spectroscopy indicated +3 oxidation state of Bi and Fe, and a reduction in unoccupied states with the increasing Bi content. This implies a modified electronic structure and oxygen vacancies. Among all the compositions, Bi_{1.05}FeO₃ has the highest BiFeO₃ phase while retaining the structural and electronic properties.

Synthesis and Structural Characterization of *h*-BN Nanocrystals: Effect of Synthesis Parameters and N₂ Environment Annealing

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Hexagonal Boron Nitride (h-BN), known as “white graphene” has attracted significant research attention due to its remarkable thermal stability, wide optical band gap (5.6 eV), mechanical strength and chemical stability. Such remarkable properties position h-BN as an ideal material for nanoelectronics, high temperature applications and energy storage devices. However, its single-phase synthesis has been challenging. In present work, a simple and cost-effective approach was developed by varying nitrogen containing precursors: urea and melamine, while using boric acid as boron source. The h-BN samples were prepared through a wet chemical route followed by annealing under nitrogen gas (N₂) atmosphere. X ray diffraction (XRD) confirmed the successful formation of h-BN nanocrystals. Field emission-scanning electron microscopy (FE-SEM), confirmed nanoparticles and nanorod morphologies by varying the synthesis protocols. The study demonstrates that the choice of precursor strongly influences crystallinity and morphology, providing a scalable and economical route for high quality h-BN suitable for advanced applications in diverse fields.

The Physicochemical and Ultrasonic Study of Clonazepam with Methanol at 303 K

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This research investigated how methanol interacts with Clonazepam, a benzodiazepine derivative at 303 K. Measurements of physicochemical properties and ultrasonic velocity provide important information about molecular association and solute–solvent interactions. For the study, clonazepam solutions in methanol at various concentrations were made. “Ultrasonic velocity (U), density (ρ), and viscosity (η)” were measured using standard experimental techniques. Various derived thermodynamic and acoustic parameters, such as “Isentropic compressibility (β_s), Acoustic impedance (Z), Shear's relaxation time (τ), and Intermolecular free length (Lf),” were computed from these experimental data. The experimental and computed findings were then analysed to estimate the kind and magnitude of solute-solvent interactions. The findings showed that when concentration rise, ultrasonic velocity and associated thermodynamic parameters systematically change. Overall, the data show that clonazepam and methanol at 303K have a strong molecular interaction. This is mostly due to the polar protic nature of methanol because of which it forms strong hydrogen bonds with the heteroatoms of clonazepam causing a large amount of solvation. A strong solute-solvent interaction with the increase in concentration is further proved from the experimental and computed data. The results imply that the presence of methanol enhances the molecular association of clonazepam.

On the Evolution of Gradient Microstructure in Hot-Rolled Titanium Subjected to Bending

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Titanium (Ti) and alloys have drawn significant attention as thin structural bioimplants over ferrous alloys owing to their high specific strength, low density, and excellent biocompatibility. To make such thin components, the material must undergo large plastic forming operations that essentially involve bending. Bending involves the complex distribution of stress and strain throughout the thickness and width direction, resulting in a heterogeneous microstructure development. In this regard, commercially pure Ti (CP-Ti) was subjected to three-point bending at an angle of 90° to observe the microstructural features developed across the thickness and width. The bend region could be distinguished as (i) inner layer, (ii) central layer, and (iii) outer layer. The microstructural features were characterized by a field-emission scanning electron microscope (FE-SEM) equipped with an electron back-scattered diffraction (EBSD) technique. The results show that the inner layer was primarily deformed by a significant fraction of twins, leading to a sharp change in texture. The outer layer is mainly deformed by slip-based deformation with a marginal change in texture development. The central layer appears to be similar to the initial coarse-grain microstructure. The present findings are essential for optimizing the processing parameters to meet the end product requirements.

Electrolyte Engineering: Role of KOH Concentration in Boosting Charge Storage of G-C₃N₄/Cr₂O₃ Nanocomposites

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The increasing global demand for renewable and efficient energy systems highlights the urgent need for high-performance, eco-friendly energy storage materials. In this work, g-C₃N₄/Cr₂O₃ nanocomposite was synthesised using the ultrasonication method and systematically evaluated in potassium hydroxide (KOH) electrolytes of varying molarity (1 M, 3 M, and 6 M) to study the role of electrolyte concentration on its electrochemical behaviour. The successful formation of the nanocomposites was verified by the XRD analysis. Structural and morphological characterisations using SEM and FT-IR confirmed uniform dispersion of metal oxide nanoparticles across the 2D matrix, promoting efficient electron–ion interaction. Electrochemical analyses, including cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS), revealed a strong dependence of performance on electrolyte molarity. The nanocomposite exhibited the highest specific capacitance of 377.6 F/g in 3 M KOH, compared to 287.7 F/g in 1 M and 158.3 F/g in 6 M at the current density of 1 A/g. These findings demonstrate that careful tuning of electrolyte molarity is essential for optimising the energy storage efficiency of nanocomposite electrodes. This study provides valuable insight into electrolyte–material interactions, advancing the design of next-generation supercapacitors aligned with environmental sustainability goals.

Epigrammatic Status of Recent advancements in the Development of Oxadiazole and its Derivatives Using Nanocatalysts

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Heterocyclic compounds are amongst the most promising and versatile classes of biologically important molecules. Oxadiazole, a five-membered heterocyclic ring containing one oxygen and two nitrogen atoms. Due to the different arrangements of the hetero atoms, oxadiazoles exist in different isomeric forms. Oxadiazole and its derivatives have attracted significant attention due to their diverse application of biological activities such as anti-cancerous, antiviral, antimicrobial, antibacterial etc. It can be synthesized by using nitriles via a 1,3-dipolar cycloaddition, reaction, *o*-acylation of amidoxime using an acid chloride or anhydride, condensation of aldehydes with hydrazides, cyclisation of hydrazides using CS₂. Oxadiazoles can be synthesized using more progressive and efficient nanoparticles as catalysts. The use of nanocatalysts is grabbing the attention of researchers owing to their more efficacy and reproducibility, low cost, reusability, ease of production, etc. ¹H NMR, FT-IR, HRMS, XRD and FE-SEM spectroscopic techniques are used for the characterization of oxadiazoles and nanocatalysts.

Sensor Technology Development and Applications in the Automotive Sector

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Sensors play a crucial role in modern vehicles providing them with a pyramid of benefits, they eventually enhance safety measures by automatically monitoring basic parameters like tire pressure and individual vehicle proximity resulting in alerting the drivers of potential disasters. Efficiency is also important and is improved through Sensors that optimize fuel consumption and performance of the engine. Materials like silicon, ceramics, and metals are commonly used due to their versatility and ability to withstand unfavourable conditions. These Sensors precisely control the diagnostics contributing to smoother operation and enhancing the life span of vehicles. Automotive sensors create a fundamental component of modern vehicles, to facilitate real-time monitoring and control of their multiple parameters enrolling the crucial perspective of vehicle performance, safety, and efficiency. The study deliberates on the core relationship between sensors and materials and their performance in the Automotive context it thoroughly excludes the critical importance of material characteristics in determining the sensor functionality and reliability. Moreover, prominent advancements in material science have shown a way to the development of innovative sensor materials. The extreme conditions while maintaining precision and reliability by testing and examining the interchange between materialistic properties and sensor performance. This study aims to provide a comprehensive understanding of how multiple characteristics influence the Design, functionality, and reliability of automotive sensors. Ultimately resulting in the enhancement of vehicle performance and equally propitious to its sustainability.

An Apotheosis Based on Apple Polysaccharides Capped with Metallic Nanoparticles for the Treatment of Gastric Ulcer

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Gastric ulcer disease remains a persistent global health issue characterized by mucosal damage caused by oxidative stress, inflammation, and microbial infection. Conventional drug therapies such as proton pump inhibitors and antibiotics often exhibit limited efficacy and cause undesirable side effects. In this study, we report an apotheosis of apple polysaccharide-capped metallic nanoparticles (MNPs) as a biocompatible and multifunctional therapeutic approach for gastric ulcer management. Apple-derived polysaccharides, rich in pectin, were employed as natural stabilizing and capping agents to synthesize silver and gold nanoparticles via a green reduction method. The resulting bioconjugates demonstrated enhanced stability, mucosal adhesion, and controlled release potential under gastric conditions. Structural and morphological characterization through UV-Vis spectroscopy, FT-IR, XRD, and TEM confirmed the successful capping and nanoscale integrity of the particles. In vitro assays revealed potent antioxidant and antibacterial activity, while in vivo studies in ulcer-induced models exhibited significant mucosal protection, decreased ulcer index, and improved histopathological recovery compared to standard treatments. The synergistic interaction between apple polysaccharides and metallic nanoparticles enhanced oxidative defense, reduced inflammation, and promoted epithelial regeneration. This study presents a sustainable, biopolymer-based nanoplatform that unites natural bioactivity with nanotechnology, providing a promising, eco-friendly therapeutic alternative for gastric ulcer therapy.

Development of High-Entropy Oxide Nanostructures for Rapid and Sustainable Amine Production

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High-entropy materials have recently emerged as a promising class of catalysts due to their high configurational entropy, which arises from structural disorder in single-phase, multi-component systems. However, the catalytic potential of high-entropy oxides (HEOs) remains relatively underexplored. In this work, we report a simple, solution-based combustion synthesis route for preparing two low-cost, transition-metal-rich multicationic oxides-positioned in the medium-entropy (HEO-4) and high-entropy (HEO-5) regimes. Rietveld refinement of powder X-ray diffraction data confirmed the formation of single-phase nanostructures with an fcc crystal lattice in both samples. Detailed morphological, size, and multicationic elemental analyses were carried out using scanning and transmission electron microscopy. The catalytic activity of these HEOs was systematically evaluated in the hydrogenation of various nitrophenol derivatives. Remarkably, HEO-5 exhibited substantially enhanced catalytic performance ($k_{app} \approx 0.5 \text{ min}^{-1}$, $\text{TOF} = 2.1 \times 10^{-3} \text{ mol g}^{-1} \text{ s}^{-1}$), achieving rapid conversion of p-nitrophenols compared to its medium-entropy counterpart ($k_{app} \approx 0.02 \text{ min}^{-1}$, $\text{TOF} = 7.2 \times 10^{-4} \text{ mol g}^{-1} \text{ s}^{-1}$). Furthermore, the reaction kinetics and thermodynamic parameters (E_a , ΔH^\ddagger , ΔG^\ddagger , and ΔS^\ddagger) were determined to provide mechanistic insights into the reduction process. Overall, this study demonstrates a rational and facile approach for designing and synthesizing high-entropy oxides as efficient, scalable catalysts for sustainable amine production.

MOF-Derived Fe-Doped MnO₂ Nanozymes with Oxidase-like Activity for Colorimetric Sensing of Hg²⁺ and Hydroquinone

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The structure and morphology of nanozymes play a pivotal role in enhancing their biomimetic catalytic behavior. In this work, we report a facile in-situ oxidation strategy to synthesize MOF-derived Fe-doped MnOx nanozymes with enhanced oxidase-like activity. The influence of Fe substitution, phase evolution, and morphological modulation on catalytic performance was systematically explored. Oxidase activity was evaluated using 3,3',5,5'-tetramethylbenzidine (TMB) as a chromogenic substrate, producing a blue oxidized product (ox-TMB) with an absorption peak at 652 nm upon oxidation. Among the prepared samples, 10% Fe-doped MnOx exhibited the highest oxidase-mimicking activity due to the synergistic contributions of optimized structure, controlled morphology, and abundant oxygen vacancies. Furthermore, the developed 10Fe-MnOx nanozyme was utilized as a dual-mode colorimetric probe for the selective and sensitive detection of Hg²⁺ and hydroquinone (HQ) in real water samples, achieving low detection limits of 0.47 μ M and 1.74 μ M, respectively. This work demonstrates a facile and scalable approach for constructing high-performance MOF-derived nanozymes, offering great promise for environmental monitoring and biochemical sensing applications.

Sustainable Electrolytes Based on Biopolymers and Biodegradable Ionic Liquid: Innovative Approach Towards Sustainable Lithium-Ion Energy Storage Devices

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Occupying a place of choice in our everyday life as energy storage devices, lithium-ion batteries are nowadays the most solicited battery on the market for many decades now. The lithium-ion battery market is continuously growing; therefore, it has to cope with regulatory sustainability requirements for batteries. The increasing demand for lithium-ion batteries in various sectors like electronics (computers, phones, smart watches, etc.), transportation (EVs, hybrid cars), and energy storage grids, besides the innovative aspect of the technology, started to raise the question of sustainability. In that direction, massive interest has been given to biopolymer-derived materials. The present work studies cellulose-based biopolymers, namely methyl cellulose (MC) and cellulose acetate butyrate (CAB), as potential electrolytes for lithium-ion batteries, and in order to improve the efficiency while remaining aligned with the sustainability aspect, ethyl ammonium nitrate (EAN), a biodegradable ionic liquid, was synthesized to plasticize our bio-based electrolytes. Based on this study, the obtained outcomes were an ionic conductivity in the range of [103 – 104] S/cm, good thermal stability above 150°C, and excellent self-healing properties. This contributes to the development efforts towards future sustainable LIBs.

Modifications Induced in the Structural, Optical, and Photocatalytic Application by Cu and Mo ions Doping in BiVO₄ Nanoparticles

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Comprehensive experiments were conducted to investigate the effects of Cu and Mo doping on the photocatalytic performance of bismuth vanadate (BiVO₄) nanoparticles. In this study, BiVO₄ nanoparticles were synthesized via the sol-gel method, Cu and Mo doped with various atomic percentage, and characterized using X-ray diffraction (XRD), Field emission scanning microscopy, Raman spectroscopy, Photoluminescence (PL) spectroscopy, UV-Vis spectroscopy, and field-emission scanning electron microscopy (FE-SEM). The XRD and Raman spectra confirmed the crystalline nature of the material and its monoclinic scheelite phase. Morphological analysis using FE-SEM revealed the formation of irregular, spherical, and rod-like shapes with sizes ranging from approximately 200 to 400 nm. PL spectroscopy was employed to examine charge recombination rates, demonstrating a significant enhancement in photocatalytic performance due to the presence of oxygen vacancies. Furthermore, the doping of BiVO₄ with Cu and Mo significantly improved its photocatalytic behavior compared to pristine BiVO₄.

Biodegradable Plastic-based Nanoadsorbents for the Removal of Methyl Green Dye from Wastewater

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Microplastics are a source of environmental concern due to their potential toxicity and prolonged persistence under natural conditions, resulting in widespread pollution across marine, freshwater, and terrestrial ecosystems. To address this concern, the present work focuses on the fabrication of nanoadsorbent viz. NA-S from biodegradable plastic straws. NA-S was analyzed using FTIR, XRD, BET, and FE-SEM + EDAX analyses. FTIR and XRD analyses of NA-S showed spectra similar to polylactic acid (PLA), confirming the presence of oxygen-containing functional groups with a semi-crystalline structure. BET analysis demonstrated surface area and average pore diameter of 9.46 m²/g and 47.96 Å, respectively, confirming the mesoporous nature of NA-S. FE-SEM analysis revealed the spherical morphology of the adsorbent particles, while EDAX showed two distinct peaks corresponding to carbon and oxygen with atomic percentages of 82.09% and 17.9%, respectively. The thermodynamics study revealed that the adsorption process was spontaneous and endothermic in nature, and it follows the Freundlich and pseudo-second-order models. A batch adsorption study was conducted to evaluate the removal efficiency of NA-S for Methyl Green dye, achieving approximately 90% removal. These findings highlight the great potential of biodegradable plastic-based nanoadsorbents for removing pollutants from wastewater.

Valorisation of Grewia Optiva Fiber for Effective Lignin Extraction and its Sustainable Use for Methyl Green Removal from Wastewater

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The study presents valorization of underutilized Grewia Optiva fiber for yielding eco-friendly lignin (GOF@L) and which has shown tremendous potential for use as adsorbent in sustainable dye remediation from wastewater. The extracted lignin showed high biogenicity with 81% C content, high surface functionality, nano-dimensional porous networked polymeric structure, exhibiting high mesoporosity to the tune of 80% with a surface area of 90.18 m²/g as confirmed via FTIR, BET, Fe-SEM, EDAX, TEM, and XRD analyses. Initial laboratory conducted batch adsorption experiments showed 63% methyl green removal within 30 mins of contact time and using 1 g/L of adsorbent. Optimization process showed >90% dye removal efficiency. The binding was monolayer and physisorption as revealed from adherence to Langmuir isotherm and pseudo-second-order kinetics model. Thermodynamic studies showed spontaneity and endothermicity for the adsorption process. Overall, GOF derived lignin is a value-added bio-material holding potential as advanced adsorbent for sustainable wastewater treatment.

Synthesis and Characterization of Antibacterial Sodium Alginate-G-N,N-Hydroxyethyl Acrylamide Films for Sustainable Biomedical Applications

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The advancement of sustainable biopolymers with superior functional and biological characteristics is crucial for modern biomedical and environmental applications. In the current study, sodium alginate-based films were created by free radical graft copolymerization of N,N-hydroxyethyl acrylamide (HEAA) using ammonium persulfate (APS) as an initiator at 80°C for 1 hour. The modification aimed to enhance the mechanical stability, surface characteristics, and antibacterial efficiency of native alginate matrices. The prepared films were characterized by Fourier Transform Infrared Spectroscopy (FTIR) to confirm grafting and chemical interactions, Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM) to evaluate surface morphology and roughness, X-ray Diffraction for determining structural order, and Thermogravimetric Analysis (TGA) for assessing thermal stability. Antibacterial activity showed notable inhibitory effects against specific bacterial strains when examined using the agar diffusion method. The results demonstrate that grafted sodium alginate films exhibit improved physicochemical and antibacterial properties, emphasising the potential for biomedical applications such as wound dressings, tissue scaffolds, and ecofriendly packaging materials, thereby contributing to sustainable material innovation in healthcare and environmental technology.

Advanced TiO₂ Composite Nanomaterials for Sustainable Pollutant Removal and Sensing

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Titanium dioxide (TiO₂) has been recognized as a benchmark photocatalyst because of its strong oxidative potential, stability, and environmental safety. However, its wide band gap and rapid electron-hole recombination limit its visible-light utilization and photocatalytic efficiency. To overcome these problem, TiO₂-based composite nanomaterials have emerged as a powerful strategy to achieve synergistic enhancement in both pollutant degradation and sensing performance. This work consolidates recent advancements in the design of TiO₂ composites incorporating metal oxides (Fe₃O₄, ZrO₂, ZnO), carbonaceous materials (graphene, CNTs), and metal-organic frameworks. These heterostructures exhibit improved charge carrier separation, band-gap tuning, and surface adsorption, enabling efficient degradation of pharmaceutical and dye pollutants such as naproxen, ibuprofen, and methylene blue under solar or visible irradiation. The presence of secondary components facilitates electron transfer pathways and enhances radical generation ($\bullet\text{OH}$, $\bullet\text{O}_2^-$), leading to accelerated photodegradation kinetics. Additionally, the modified surface chemistry of TiO₂ composites provides sensitive and selective optical or electrochemical responses toward analytes, highlighting their dual applicability in environmental remediation and chemical sensing. The comparative analysis emphasizes structure-property relationships, reaction mechanisms, and the role of interface engineering in achieving multifunctionality. Overall, TiO₂ composite nanomaterials represent a sustainable and scalable platform for integrated photocatalytic-sensing systems addressing emerging environmental challenges.

***in-situ* Synthesis of HKUST-1 inside Biochar Pores and its Synergistic Effects on The CO₂ Adsorption Properties**

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The rapid escalation of anthropogenic CO₂ emissions necessitates sustainable and cost-effective carbon capture solutions. Biochar, while renewable and low-cost, suffers from limited porosity and adsorption efficiency, whereas metal-organic frameworks (MOFs) such as HKUST-1 possess high surface areas and tunable chemistry but face challenges of stability, scalability, and synthesis cost. In this work, an in-situ synthesis approach was employed to integrate HKUST-1 within *Citrus limetta* peel biochar (CLPB) to prepare a composite (HKUST-1@CLPB) with improved CO₂ adsorption properties. The materials were synthesized and characterized using PXRD, FTIR, SEM, BET surface analysis, and TGA, followed by high-pressure CO₂ adsorption isotherms at 25 °C. Pristine CLPB exhibited negligible porosity (surface area 0.12 m²·g⁻¹) with low CO₂ uptake (1.54 mmol·g⁻¹ at 10 bar), whereas HKUST-1 showed higher surface area (539.01 m²·g⁻¹) and CO₂ capacity (4.83 mmol·g⁻¹). The HKUST-1@CLPB composite displayed a significant enhancement over CLPB, with surface area increased to 132.5 m²·g⁻¹, micropore volume to 0.048 cm³·g⁻¹, and CO₂ uptake to 2.03 mmol·g⁻¹ at 10 bar, corresponding to a 31.3% improvement. Structural and spectroscopic analyses confirmed the successful incorporation of HKUST-1 within the biochar matrix, with interfacial interactions modifying adsorption environments. The results demonstrate that in-situ MOF integration effectively upgrades waste-derived biochar into a functional sorbent by combining structural porosity with surface functionalities. This study provides critical insights into structure-property-performance relationships in MOF-biochar composites and underscores their potential as sustainable, scalable materials for CO₂ capture applications.

Investigation of Radiation Tolerance in Ceramic Composite and Non-Composite Materials

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Materials exposed to extreme environments, such as those found in nuclear reactors and outer space, face significant challenges due to intense radiation and extreme temperatures, which can degrade their properties and shorten their operational lifespan. Enhancing the radiation tolerance of these materials is crucial for improving their performance in such harsh conditions. Yttria-stabilized zirconia (YSZ) is well-regarded for its radiation tolerance, making it a candidate for nuclear applications.^{1,2,3,4} However, its low thermal conductivity limits its effectiveness, as thermal conductivity is a key factor in mitigating radiation-induced damage. To address this limitation, we explore the potential of a YSZ-MgO composite, which combines YSZ with a material of higher thermal conductivity, potentially enhancing overall radiation tolerance. Additionally, the presence of heterointerfaces in the composite may serve as effective defect sinks, further improving its resilience. The study investigates the radiation tolerance of YSZ-MgO composites subjected to 400 keV Kr ion irradiation at room temperature and 80 MeV I ion irradiation at both room temperature and 700°C. Grazing Incidence X-Ray Diffraction (GIXRD) analysis indicates that the YSZ-MgO composite exhibits less microstructural damage compared to single-component YSZ. X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) analyses revealed that the Zr atoms in all samples exhibit negligible changes in binding energy and oxidation state. In contrast, the composite samples show a noticeable shift in the binding energy of Mg atoms after irradiation, which is consistent with the corresponding shift observed in O atoms. Notably, the samples demonstrated reduced damage in high-temperature irradiations with 80 MeV I ions compared to room temperature irradiations. Further insights from Raman spectroscopy, Extended X-ray Absorption Fine Structure (EXAFS) analysis, and theoretical thermal simulations will be presented to elucidate the underlying mechanisms contributing to the observed radiation response.

Synthesis and Characterization of *h*-BN and Laser Induced Graphene Based Nanocomposites

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Hexagonal boron nitride (*h*-BN) are highly porous, crystalline hybrid materials. Hexagonal boron nitride stands out due to their low cost, environmental friendliness, low toxicity, and water stability. Their versatility and high porosity make them suitable for a wide range of scientific and industrial applications. In this work, *h*-BN has been synthesized using chemical method. The laser induced graphene (LIG) was prepared using CO₂ laser irradiation over polyimide sheet with a power of 5 W and laser scribing speed of 80 mm/s. The nanocomposites were also prepared using laser induced method by dispersing the *h*-BN and ethanol solution over LIG synthesized polyimide sheet in different weight ratios. The prepared nanocomposites were characterized using X-ray diffraction (XRD), Raman spectroscopy, Fourier transform infrared spectroscopy (FTIR) and Scanning electron microscopy (SEM). The characteristic peaks of *h*-BN in XRD confirms the formation of nano-composites. Raman spectroscopy conveyed the D, G and 2D bands of Graphene along with the vibrations of *h*-BN. The FTIR suggested the B-N, B-O, C-N and C-B related bonds along with graphene-based carbon bonds which further confirms the nanocomposite formation.

Keywords: Hexagonal boron nitride (*h*-BN); Fe-MOF; Carbon material; Raman spectroscopy.

Biobased Thiol-Acrylate Vitrimers for Light-Based 3D Printing with Programmable Healing and Shape Recovery

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Dynamic covalent chemistry has opened new pathways for designing polymer networks that can repair damage, be reshaped, and undergo controlled reconfiguration. Incorporating biobased feedstocks into such systems further strengthens their sustainability profile while maintaining functional performance. Combining these elements within additive manufacturing platforms allows the production of adaptable materials with lower environmental burdens. This work presents the development of renewable thiol-acrylate vitrimer formulations engineered for light-based 3D printing, with a focus on soft, reconfigurable devices exhibiting self-healing and programmable shape recovery. The resin system integrates acrylated epoxidized soybean oil (AESBO), a glycerol-derived diluent, and a multifunctional thiol to generate networks with tunable viscoelasticity and efficient bond-exchange behavior. The hydroxyl-ester linkages formed during polymerization enable catalyzed transesterification at elevated temperatures when a tin catalyst is introduced, allowing the printed structures to reorganize without loss of integrity. Dynamic mechanical analysis demonstrates that varying the AESBO fraction strongly influences the glass transition temperature, stiffness, and overall network mobility. Stress relaxation studies confirm rapid bond exchange kinetics, with the materials releasing approximately 63% of internal stress within 3.6 minutes at 200 °C, thereby facilitating self-healing and shape reformation. The materials showed promising healing, shape memory, degradability, and reprocessing capabilities, highlighting its potential for use in soft active devices and soft robotics applications.

One-Pot Synthesis of Naphthopyranopyrimidines by Green Catalyst

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This work uses sugarcane juice as a heterogeneous catalyst to synthesize naphthopyranopyrimidines and their derivatives in an environmentally friendly, solvent-free manner. Three components—benzaldehyde, β -naphthol, and 1,3-dimethylbarbituric acid—condense in a single pot at 75°C with 20 mol% sugarcane juice, producing substantial yields in a brief amount of time. Since no product production was seen in the absence of sugarcane juice, control studies validated its crucial catalytic role. Several benzaldehydes with electron-donating and electron-withdrawing groups were used to test the protocol's breadth; they showed broad compatibility and produced a variety of naphthopyranopyrimidine derivatives. Using mass spectroscopy, ¹HNMR, and ¹³CNMR, the products were described. This environmentally benign and effective method for heterocyclic synthesis demonstrates the potential of renewable bio-catalysts in green chemistry.

Efficacy of the Langmuir Hinshelwood Hougen Watson Kinetics in Aspen Plus Modelling of Catalytic Transesterification to produce FAME Biodiesel

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The persistent rise of global temperature and environmental pollution as a result of greenhouse gas emissions is a primary concern for mankind. In addition, the depletion of natural energy resources like coal, crude oil, and natural gas is occurring rapidly, raising the issue of an energy crisis in the near future. Therefore, the dependence on renewable fuel sources like Fatty Acid Methyl Ester (FAME) biodiesel is a must. FAME biodiesel is produced via catalytic transesterification, which is considered a green process. However, the scale-up of the process requires the use of an effective simulation tool, such as Aspen Plus, and the incorporation of proper reaction kinetics. In the present study, models for the production of FAME biodiesel are developed using Langmuir-Hinshelwood-Hougen-Watson (LHHW) kinetics and compared with other kinetic models, such as the Powerlaw model. It is observed that LHHW kinetics can elevate the conversion efficiency of transesterification up to 96% with a significant yield of 7.5 kg/hr. In contrast, the power law does not fit the heterogeneous catalytic transesterification process and brings only 21% conversion efficiency.

Optimization of Thermoelectric Properties of BiSbTe₃ Single Crystal through Se substitution

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Bismuth antimony telluride (BiSbTe₃) has been extensively studied due to its novel thermoelectric characteristics, exhibiting superior thermoelectric performance at ambient temperature (300K). This study aims to understand the impact of substituting Selenium (Se) at the site of Tellurium (Te). We present the thermoelectric and electrical transport characteristics of BiSbTe_{3-x}Se_x by varying x. The Se-substituted single crystal of BiSbTe_{3-x}Se_x ($0 \leq x \leq 0.05$) were synthesized using modified Bridgman technique and its transport properties are measured. The RT measurement reveals the metallic nature, whereas the positive slope of ST suggest that the dominant carriers are holes (p-type) for both single crystals. The lowest substituted sample (x=0.05) has hugely increased power factor of around $\sim 583\% \mu\text{W}/\text{m}\cdot\text{K}^2$ at 300K. This is because resistivity ($\rho\text{-m}\Omega\cdot\text{m}$) has decreases about 62.5% and the Seebeck Coefficient (S- $\mu\text{V}/\text{K}$) of Se substituted sample has increased by 60% as compare to pristine sample (x=0). The enhanced in PF is possible because the pockets of the carriers are getting closer to the fermi level, carrier concentration increases. Its high efficiency is considered for fabrication of thermoelectric devices and thermoelectric generators (TEGs).

Computational Modelling on Electrochemical Performance of Jute Waste Derived Activated Carbon as Supercapacitor

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For sustainable development, valorization of lignocellulosic industrial waste into activated carbon emerges as a promising approach. In the present research, jute waste is utilized, which shows potential for supercapacitor application in terms of amorphous nature of carbon having a specific surface area (SSA) of 1100 m²/g as confirmed by BET isotherm and RAMAN spectral analysis reflected characteristics D and G peaks at 1300 cm⁻¹ and 1500 cm⁻¹ respectively indicating graphitic nature of the prepared carbon. Electrochemical performance was evaluated in a symmetrical 2032 supercapacitor full cell which delivered specific capacitance up to 70 F/g at a constant current of 1mA at 0.5mA/cm². Computational modelling methods including Density functional theory (DFT) and Molecular dynamics (MD) are significant for the exploration of charge storage mechanism. The present study is designed to use DFT for monitoring how specific capacitance is governed by different distribution of pore size and volume and further determination of Quantum Capacitance from DOS for better visualization of the overall capacitance. The overall study emphasizes a detailed understanding on utilization of lignocellulose rich jute waste as a potential substrate for development of active carbon in line with the waste to energy perspectives.

Cost-Effective Lifepo4 Cathodes using Fe³⁺ Precursors through Aqueous Xerogel Route With in situ Carbon Coating

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Lithium Iron Phosphate (LFP) is considered one of the most reliable cathode materials for lithium-ion batteries, yet the widespread use of Fe²⁺ precursors limits its scalability due to high cost and poor stability. We demonstrate an aqueous xerogel strategy to synthesize single-phase, in situ carbon-coated LFP using ferric nitrate as the iron source. Fe³⁺ ions were reduced to Fe²⁺ ions by ascorbic acid and stabilized with EDTA. The resulting nanoscale LFP particles exhibit high crystallinity with conductive carbon networks, as confirmed by PXRD, Raman, and HRTEM analysis. Electrochemical testing revealed an initial discharge capacity of 140.40 mAh g⁻¹ at 0.1C, with excellent rate performance of 60.63 mAh g⁻¹ at 10°C and capacity retention of 68.39% after 300 cycles. The cells also demonstrated outstanding rate capability at high current densities (0.05-5.3 mA cm⁻²). This study highlights the potential of utilizing low-cost, abundant Fe³⁺ salts as precursors for scalable and green synthesis of LFP for application in high-performance lithium batteries.

SOFC-GT Hybrid CHP Systems: An Aspen Based Study towards Thermoeconomic Outlook

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The Solid Oxide Fuel Cell (SOFC) technology is one of the prominent pillars of the new era of green energy because of its high temperature internal reforming ability. This allows SOFC to use carbonaceous fuels. However, efficient high-temperature operation requires secondary devices such as afterburners, heat-exchanging recuperators, and fuel re-circulators in a Combined Heat and Power (CHP) plant during practical deployment. The following study examines various literature and in-house based plant designs to analyse operational obstacles. These include maintaining high temperature, fuel utilisation and system efficiency. Various permutations were analysed to characterize the causes. The most prominent limitation was identified as the division between electrical (ΔG) and thermal energy ($T\Delta S$). The use of CHP-load devices, such as a Gas Turbines (GT), allows for the sensible heat recovery. The potency of carbonaceous fuels such as commercial-grade syngas and methane was also explored. The differences in their thermodynamic reactions significantly influences the system's operation. Various models about the thermodynamic breakdown of syngas and methane were constructed to study the energy balance. The combination of these resulted in a trade-off between high efficiency and fuel flexibility. The study highlights the immense potential inherent in such hybrid systems to attain high-grade and sustainable energy.

Structural Insight into Mo-Doped Sr-Fe-O Based Double Perovskite via in-situ High-Temperature XRD: A Correlation of Mo Doping with Electrochemical Activity in RSOCS

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The development of highly active and redox stable oxygen electrode is critically needed for the advancement of Reversible Solid Oxide cells (RSOCs). This study investigates the structural and electrochemical effects of Molybdenum (Mo) doping concentration in the Sr-Fe-O based double perovskite system (15% - 25%) to identify the optimum composition for enhanced performance. High-temperature X-ray diffraction (HT-XRD) technique was primarily used to understand in-situ structural insights, phase stability, lattice parameter evolution, and potential phase transitions as a function of both Mo content and temperature. This study also reveals a critical dependence of the oxygen vacancy concentration and thermal expansion behaviour on the Mo doping, which directly correlates with the material's electrochemical activity. Electrochemical testing, including impedance spectroscopy and polarization measurements, confirmed that an optimum Mo concentration (25%) lowers the resistance and improves oxygen kinetics (ORR, OER) for RSOCs. Furthermore, after cell testing, scanning electron microscopy of the best-performing composition provided a deeper understanding of the material's operational stability, revealing minimal structural degradation and confirming the structural stability imparted by the optimized Mo concentration. These findings establish a direct structure-performance nexus, highlighting the power of HT-XRD in guiding the rational design of transition metal oxide materials to get high electrochemical performance.

Ce_{0.25}Zr_{0.75}O_{2-δ} Catalyst Integration for Low-Resistance & Durable SOEC Fuel-Electrodes

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Solid oxide electrolysis cells (SOECs) are among the most promising technologies for sustainable hydrogen production owing to their high energy conversion efficiency. However, further enhancement of electrolysis current density is essential to meet practical application demands. In this work, we report a novel SOEC fuel-electrode configuration based on cerium oxide, renowned for its redox activity and ability to disperse metal nanoparticles, with Zr incorporation to significantly improve ionic conductivity. The resulting NiO-YSZ-Ce_{0.25}Zr_{0.75}O_{2-δ} fuel-electrode achieves a polarization resistance of 0.0158 Ω·cm² at 800 °C and 1.5 V. Moreover, the current density reaches 1.057 A·cm⁻², nearly three times higher than that of a conventional NiO-YSZ scaffold (0.384 A·cm⁻²). The cell further demonstrates stable steam electrolysis at ~1.0 A·cm⁻² and 800 °C under 1.5 V, corresponding to a hydrogen generation flux rate of 0.44 NL·h⁻¹·cm⁻². These results highlight the potential of Ce–Zr oxide as a catalyst for next-generation SOECs fuel-electrode with enhanced performance and durability.

Silver Nanowires Assisted Waste-Derived rGO and PPy (AgNW/WrGO/PPy) Composite for High Energy Density Supercapacitor Electrode

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Supercapacitors are recognized as vital energy storage devices due to their high power density, fast charge/discharge capabilities, and long cycle life. Significant advances in materials science, especially in graphene, conducting polymers, and highly conductive silver nanowires (AgNWs), have greatly improved their performance and increased their role in sustainable energy technologies. This study presents the synthesis of Ag nanowires (AgNWs), rGO prepared from solid plastic waste (WrGO), and polypyrrole (PPy), referred to as AgNW/WrGO/PPy composite, as a highly conductive electrode material for supercapacitors. The composite offers a low-cost, eco-friendly option for supercapacitor electrodes, creating a strong, highly conductive network. Structural analyses using XRD, FE-SEM, and FTIR confirmed the formation of AgNW/WrGO/PPy composite. XRD showed sharp peaks matching AgNWs and a hump around 25°, characteristic of WrGO/PPy. SEM images revealed that WrGO/PPy effectively coats the AgNWs via intermolecular interactions. Electrochemical tests showed that with a 10 wt% loading of AgNWs, the composite achieved a high specific capacitance of 353.4 F g⁻¹ at 0.5 A g⁻¹. It also delivered an energy density of 49.1 Wh kg⁻¹ and a power density of 250 W kg⁻¹, and the electrode retains 87.16% of its initial capacitance after 5000 cycles, highlighting its potential as a sustainable, eco-friendly, and cost-effective material for supercapacitor electrodes in energy storage applications.

Surfactant-Assisted Nickel Ferrite Electrodes with Superior Coulombic Efficiency for Supercapacitors

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The ever-increasing demand for energy has led to the exploration of energy harvesting from different sources, such as batteries, fuel cells, and electrochemical capacitors or supercapacitors. Nickel ferrite nanoparticles synthesized using a surfactant-assisted co-precipitation method demonstrate significant changes in their electrochemical properties, making them promising candidates for supercapacitor applications. When surfactants such as polyethylene glycol (PEG), oleic acid etc. are used during synthesis, they act as capping agents, effectively modifying particle growth, reducing agglomeration, and controlling particle size. XRD analysis confirms that all synthesized samples possess a single-phase cubic spinel structure, with variation in the structural parameters depending on the surfactant used. Electrochemical characterization shows that surfactant-assisted nickel ferrite, specifically NiFe₂O₄@PEG, achieves an impressive specific capacitance (1230.25 F/g), energy density (27.33 Wh/kg), and coulombic efficiency (89.11%) at 1 A/g in aqueous 3M KOH electrolytes, greatly outperforming native and other assisted nickel ferrite nanoparticles. These enhancements are due to the reduced and uniform particle size, which directly improves charge storage performance and places surfactant-assisted nickel ferrite as an advanced electrode material for high-performance energy storage devices.

B Site Engineered High Entropy Perovskite as Promising Cathode for Solid Oxide Fuel Cell Applications

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High Entropy material-based perovskite oxides are the emerging materials in the field of solid oxide fuel cell (SOFC) applications having multiple cations engineered B site enhancing the catalytic property as well as electrochemical performance. The nanosized La_{1-x}Sr_x(Fe Mn Ni Cr Co)O_{3- δ} (LSHEO) powder was synthesized via L-Alanine assisted Solution Combustion Synthesis for $x=0.1, 0.3, 0.5$. The room temperature powder XRD revealed the quasi-cubic phase of LSHEO for $x=0.3$ and rhombohedral for the other two ($x=0.1, 0.5$) composition. The microstructural analysis from SEM images of the samples shows spherical morphology in agglomerated form having grain size of 150-200 nm. The HR-TEM images revealed the fringe width which was correlated with the lattice parameters obtained from XRD data. The Thermal Expansion coefficient (TEC) was conducted for the samples using high temperature dilatometer which revealed that they have values in the range of $13-15 \times 10^{-6} \text{ K}^{-1}$ which is close to that of the standard electrolytes for SOFC applications like YSZ and GDC i.e., $10-12 \times 10^{-6} \text{ K}^{-1}$ at 600-800°C indicating good thermal compatibility. The four-probe DC conductivity test shows conductivity of the sample in the range of 100-200 Scm^{-1} suggesting good mixed ionic and electronic conductivity (MIEC). The variation in the Sr content plays an important role in creating oxygen vacancy and enhances the carrier charge mobility and thus the interplay of the synergistic effect of the B site cation comes into play. The oxygen adsorbed and lattice oxygen play a dominating role in determining the reaction kinetics of the air electrode material which was compared from XPS. The Electrochemical impedance spectroscopy suggests that the LSHEO for $x=0.3$ has low polarization resistance $0.2 \text{ }\Omega\text{-cm}^2$ at 800°C. The overall material characteristics suggest that the La Sr based high entropy perovskite oxide system are promising materials for air electrodes in Intermediate temperature solid oxide fuel cell (IT- SOFC).

Design and Development of Perovskite Based Nanocomposite for Sustainable Energy Storage

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The rapid industrial and technological growth has intensified global energy demands, urging the transition from conventional fossil fuels to renewable and sustainable alternatives. Among various storage technologies, supercapacitors have gained prominence for their excellent power density, fast charge-discharge capability, and long operational lifespan. Performance of energy storage devices is strongly influenced by the structural and electrochemical properties of the electrode materials. In this context, perovskite-based nanocomposites offer immense potential owing to their tunable electronic structure, high redox activity, and robust chemical stability. The present study focuses on the design and development of nanostructured perovskite-based composites synthesized via an ultrasonication-assisted method to achieve uniform dispersion, enhanced surface area, and improved conductivity. The synthesized materials were characterized using various analytical techniques, including FTIR, UV-DRS, SEM-EDX, XRD, and TGA-DTA. Their electrochemical behavior was further evaluated through cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy under different electrolyte conditions. This study aims to develop cost-effective, efficient, and stable perovskite-based electrodes for sustainable electrochemical energy storage application.

Impact of Aqueous Electrolytes on the Electrochemical Performance of Nitrogen-Doped Laser-Induced Graphene for Supercapacitors

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With the growing demand for energy and increasingly pressing environmental issues, there has been an increased emphasis on energy storage solutions such as supercapacitors (SCs), which are known for their high power density, durability, and long lifespan. Laser-induced graphene (LIG) has emerged as a promising material for SCs because of its high porosity and cost-effectiveness. Introducing heteroatoms into LIG is a novel strategy in energy storage. This study examined the synthesis of nitrogen-doped LIG (NLIG) and the effect of different electrolytes on its electrochemical properties. The process begins with the use of a CO₂ laser to irradiate a polyimide sheet, resulting in the formation of LIG. Subsequently, a urea solution was uniformly applied to the LIG and dried on a hot plate, followed by another round of laser irradiation to incorporate nitrogen atoms into the LIG. Structural analysis of the samples was performed using Raman spectroscopy and X-ray diffraction, while morphological analysis was conducted using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). X-ray photoelectron spectroscopy (XPS) confirmed the successful integration of nitrogen atoms into the LIG lattice, as evidenced by the presence of pyrrolic N, pyridinic N, and graphitic N. The electrochemical performance of NLIG was tested in various electrolytes, including KOH, NaOH, and Na₂SO₄ using a 3-electrode system. The electrode achieved a maximum areal capacitance of 68 mF/cm² at a current density of 0.3 mA/cm², demonstrating impressive energy storage capabilities with an energy density of 5.31 μWh/cm² and power density of 112.5 μW/cm² in a 1 M KOH solution. This study highlights the impact of electrolytes on the electrochemical performance of NLIG, providing a pathway for the production of high-performance SCs.

Role of Na Incorporation in Enhancing the Energy Storing Capabilities of Mn₂O₃ Nanostructures for a Symmetric Supercapacitor Device

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The rising demand of energy with the constant increase in population brings out the need for advanced energy storage systems like supercapacitors and batteries. Supercapacitors with their balanced energy and power densities dominate other available devices. Electrodes determine the performance of a supercapacitor. Metal oxides, specifically the ones with various oxidation states, garner major attention of researchers to develop high performance electrodes for supercapacitors. Among different metal oxides, manganese-based oxides like Mn₂O₃ are interesting due to the range of various oxidation states of Mn, which increases the redox activities. This work focuses on Na incorporation in Mn₂O₃ to further enhance its electrochemical performance, as Na⁺ ions facilitates ion transportation. NaMnO₂ nanostructures were synthesized by conventional solid-state approach and characterised by XRD, FTIR, SEM, EDS to determine the structural and morphological properties. Electrochemical measurements were carried out by CV (Cyclic Voltammetry), and Galvanostatic Charge-Discharge (GCD). The maximum specific capacitance from CV was 360.9 F/g at a 5 mV/s scan rate. GCD profiles also indicated pseudocapacitance. For real world applications, a symmetric supercapacitor was fabricated in a Swagelok assembly which retained 75% of its initial capacitance after 10,000 GCD cycles and a high energy density of 64 Wh/kg was achieved. These results demonstrate NaMnO₂ as a promising material for supercapacitor devices.

Electrochemical Performance of Copper Sulfide Nanoparticles Synthesized by Green Approach using *Urtica Diocia* Leaves Extract

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Copper sulfide is known to exhibit different phases ranging from CuS (covellite) and Cu₂S (chalcocite). Copper sulfide, depending upon the formed phases, has wide applicability in energy storage, photocatalysis, solar cells, sensors etc. In the present study, copper sulfide nanoparticles are deposited by hydrothermal technique by using *Urtica Diocia* leaves extract as a solvent. Formation of copper sulfide nanoparticles having average crystallite size of about 11.47 nm was confirmed by X-ray diffraction analysis. The synthesized copper sulfide nanoparticles was found to show a wide absorption band in the visible region. From the synthesized copper sulfide nanoparticles, electrodes are prepared onto graphene by spin coating technique for investigating electrochemical performance. The prepared copper sulfide electrodes showed pseudocapacitive behaviour having specific capacitance of about 95 F/g with the scan rate of 5 mV/s. Many redox peaks are seen in the CV curves indicating presence of mixed phase copper sulfide nanoparticles.

Decoding the Electrochemical Dynamics of Co-MOF Electrodes in Alkaline Electrolytes for Energy Storage

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Energy storage devices play a crucial role in addressing the growing global demand for efficient and sustainable energy solutions. Among these, supercapacitors have emerged as promising candidates owing to their high power density, rapid charge–discharge capability, and excellent cycling stability. In this work, Cobalt-based Metal–Organic Frameworks (Co-MOFs) were investigated as electrode materials due to their large surface area, tunable porosity, and redox-active cobalt centers that enhance energy storage performance. The main objective of this study is to compare the electrochemical performance of Co-MOF electrodes in KOH and NaOH electrolytes, emphasizing the influence of electrolyte type and molarity on charge storage behavior. The Co-MOF was synthesized via a hydrothermal method using benzene-1,3,5-tricarboxylic acid (BTC) as the organic linker. X-ray Diffraction (XRD) analysis revealed prominent peak at 10.89° , confirming the crystalline MOF structure, while Fourier-transform infrared spectroscopy (FT-IR) exhibited metal–oxygen–hydrogen vibrations at 648 and 511 cm^{-1} , indicating Co–OH bonding. UV–Vis DRS analysis showed a band gap of 2.86 eV, signifying strong electronic interaction between Co ions and BTC linkers, which favors charge mobility and redox activity.

Electrochemical evaluation was conducted using Cyclic voltammetry (CV), Galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS) in a three-electrode configuration. In 1M KOH, the Co-MOF electrode exhibited distinct redox activity, delivering a specific capacitance of 379.31 F g^{-1} from CV curves and 317.86 F g^{-1} from GCD measurements, demonstrating efficient charge storage and stable electrochemical behavior with an energy density of 11.04 Wh kg^{-1} and 98% coulombic efficiency after 10,000 cycles. In contrast, 1M NaOH exhibited the highest performance, achieving a specific capacitance of 780.31 F g^{-1} from CV and 1147.2 F g^{-1} from GCD at 1 A g^{-1} , along with an energy density of 21.04 Wh kg^{-1} at a power density of 125 W kg^{-1} . The superior electrochemical response in NaOH demonstrates that the electrolyte composition significantly influences ion transport and redox reactions, establishing NaOH as the most suitable electrolyte for enhancing the performance of Co-MOF-based supercapacitor electrodes.

Role of Hierarchical Porosity in Biogas Upgradation using Activated Carbons Derived through Different Activation Methods

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The rising global energy demand and the transition toward renewable energy systems have intensified interest in biogas as a sustainable energy resource. However, the presence of CO₂, N₂, and other impurities in raw biogas reduces its calorific value and limits its direct utilization, necessitating effective upgrading and purification. This study investigates the influence of different activation methods on the surface, structural, and adsorption properties of *Solanum nigrum*-derived activated carbons for selective CO₂ removal from biogas. The biomass was activated by three chemical agents (ZnCl₂, H₃PO₄, and KOH) and one physical route (CO₂) under optimized conditions. The resulting samples were characterized using BET, FTIR, FE-SEM, and XRD techniques, and their adsorption behavior toward CO₂, CH₄, and N₂ was evaluated using high-pressure adsorption isotherms. SNH0.5 exhibited the highest CO₂ uptake (5.72 mmol g⁻¹ at 1000 kPa) due to its hierarchical micro-mesoporous structure and polar surface functionalities. IAST-based adsorption selectivity for CO₂/CH₄ separation followed the order SNH0.5 > SNCO2 > SNZ0.6 > SNK1.0. Simulation studies confirmed the predominance of van der Waals interactions in CO₂ binding. The findings demonstrate that tuning the hierarchical porosity of biomass-derived carbons is an effective strategy for enhancing adsorption selectivity and advancing sustainable biogas upgrading technologies.

Effect of electrolytes on the electrochemical performance of MWCNT/MXene nanocomposite as electrode material for supercapacitor applications

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This study focuses on the synthesis and electrochemical evaluation of MWCNT/MXene nanocomposite as a high-performance electrode material. The ultrasonication approach was used in this study to synthesize MWCNT/MXene nanocomposite. The synthesized samples were characterized to investigate their potential as supercapacitor electrode materials. XRD was used to determine the structural properties of the MWCNT/MXene nanocomposites at 2θ values of 8.90° and 25.87° . Characteristic peaks of MWCNT/MXene can be seen in the Raman spectra at 1344 cm^{-1} and 1582 cm^{-1} , assigned to the D and G bands, whereas EG and Eg bands of MXene were observed at 395 cm^{-1} , 510 cm^{-1} , and 632 cm^{-1} , respectively. Further imaging via Scanning Electron Microscopy (SEM) provided visual evidence of the accordion like morphology, confirming their sheet structure along with MWCNTs having tubular morphology. The electrochemical performance of the MWCNT/MXene based electrode was investigated in five different aqueous electrolytes that is H_2SO_4 , KOH, Na_2SO_4 , KCl, and NaOH. A comprehensive set of tests, including Cyclic Voltammetry (CV), Galvanostatic Charge-Discharge (GCD), and Electrochemical Impedance Spectroscopy (EIS), was employed. Our findings demonstrate that the electrolyte plays a decisive role in the capacitive behaviour. The MWCNT/MXene electrode in 1 M KOH electrolyte exhibited superior performance, achieving the highest specific capacitance among all tested electrolytes. Specifically, values of 154.23 F/g at a scan rate of 2 mV/s (from CV) and 145.83 F/g at a current density of 1 A/g (from GCD) were recorded within a stable voltage window. In conclusion, this work not only successfully synthesizes and characterizes MWCNT/MXene nanocomposite but also provides a comparative analysis of their efficacy in various electrolytes, clearly showing 1 M KOH as the optimal aqueous electrolyte for maximizing the capacitive performance of MWCNT/MXene based supercapacitors.

Versatile g-C₃N₄ electrode design for high-performance supercapacitor and water-splitting applications

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We have entered a new era of energy consumption due to the rapid rise of contemporary society, and research on cutting-edge energy conversion and storage technologies has been promoted globally. Electric energy is becoming more and more prevalent in contemporary society as a clean, ecological, and efficient energy source. The electrochemical conversion of hydrogen and oxygen has advanced significantly in recent decades, and electrocatalytic total water splitting is capable of producing hydrogen, a clean energy source with much interest. Furthermore, supercapacitors have a high ability for any sort of energy storage device. Even said, there is still much space for advancement in the supercapacitor's comparatively low energy density. So, this work focuses on bi-functional electrodes for energy conversion and storage. In this study, graphitic carbon nitride was synthesised using a different precursor, such as urea (gCNU) and melamine (gCNM), as well as acid-treated graphitic carbon nitride (gCNMT). The goal was to investigate the enhanced uses of these materials in alkaline electrocatalysts and aqueous supercapacitors. Different methods are used to characterise materials, including X-ray diffraction (XRD) to determine crystalline nature, Fourier-transform infrared spectroscopy (FT-IR), field emission scanning electron microscopy (FE-SEM) to determine morphology, ultraviolet diffuse reflectance spectroscopy (UV-DRS) to determine bandgap and photoluminescence. The electrochemical characteristics of all three materials were investigated using three electrode configurations in a 1.0 M KOH electrolyte. All materials exhibit pseudocapacitive behaviour with a charge storage mechanism governed by maximum diffusion. Out of the three, gCNMT has the highest specific capacitance of 370 F/g at a scan rate of 2 mV/s and 390 F/g with a current density of 1.0 A/g. It also has an energy density of 40.28 Wh/kg at a power density of 810 W/kg. These properties suggest that acid-treated graphitic carbon nitride is suitable for future energy storage devices. The gCNMT electrocatalyst exhibited the lowest overpotential (40 mV) and Tafel slope (125 mV/decade) for the hydrogen evolution reaction (HER). Furthermore, the gCNMT electrocatalyst exhibited a low overpotential (264 mV) and the lowest Tafel slope (62 mV/decade) for oxygen evolution reaction (OER). Among all three, gCNMT obtains the highest double-layer capacitance (C_{dl}) of 11.6 mF and the highest electrochemical surface area (ECSA) of 290 cm². This study indicated that the acid-treated graphitic carbon nitride is extremely favourable for aqueous supercapacitor and alkaline electrocatalyst (OER and HER) applications.

Valorization of Medical Plastic Waste via Thermochemical Conversion for Hydrocarbon Fuel Production

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The rapid increase in medical plastic waste (MPW), including syringes, PPE coverall, and other disposable medical items, poses a significant environmental challenge due to its non-biodegradable nature and potential health hazards. Conventional disposal practices such as incineration and landfilling contribute to greenhouse gas emissions and toxic residue formation, making sustainable alternatives imperative. In this study, the thermochemical conversion of medical plastic waste into hydrocarbon fuels via pyrolysis was investigated as a sustainable strategy for waste minimization and energy recovery. The feedstock was characterized using thermogravimetric analysis (TGA) and Fourier-transform infrared spectroscopy (FTIR). The TGA profile revealed major degradation between 350°C and 500°C, indicating suitable thermal stability for pyrolytic processing. FTIR analysis confirmed the presence of polypropylene as major constituents, making the waste composition favorable for hydrocarbon fuel production. Non-catalytic pyrolysis was performed in a fixed-bed reactor at temperatures ranging from 350°C to 500°C. The optimal yield was achieved at 450°C, producing a liquid fraction rich in hydrocarbons. FTIR analysis of the obtained oil exhibited aliphatic and aromatic bands, confirming its potential as a conventional fuel substitute. This study demonstrates that medical waste can be effectively converted into valuable fuel-like products, providing an environmentally sustainable pathway aligned with circular economy principles. The process not only reduces the burden of hazardous medical waste but also contributes to the sustainable production of alternative fuels, supporting global energy and environmental sustainability goals.

Thermal And Radiative Analysis of a Crude Oil Tank for Boil-Over using ANSYS Fluent

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Boil-over is one of the most catastrophic phenomena that occurs in a crude oil tank. It is the ejection of hydrocarbon due to the vaporization of the water sub layer inside the tank. It leads to financial and production loss, structural damage, major environmental concern like ecological disbalance, air pollution and a threat to human life. This study presents an analysis of the thermal and radiative properties of a crude oil storage tank which undergoes boil-over using ANSYS Fluent. A three-dimensional tank model replicating TO11 of the Milford Haven boil-over incident was developed. It includes multiphase interactions, combustion dynamics and radiative heat transfer. Three models VOF Multiphase, DO (Discrete Ordinates) radiation model and Species Transport + Eddy Dissipation Combustion models were used. The VOF model was used to capture the immiscible oil and water interface, the species transport with eddy dissipation model simulated the turbulent combustion and the DO model was used to calculate heat flux in the flame zone. The results show Oil layer temperature rising to 180-230 °C, and the water layer approached boiling 95-105 °C thereafter the rapid vaporization triggered the boil-over. The surrounding air temperatures stabilized at 295–305 °K, flame core temperatures reached till 1300–1500 °C with radiative intensities up to 190 kW/m². The simulation showcased the three stages of the boil-over, the oil heating up, formation of vapour at the oil water interface and the ejection of oil. The findings strongly correlate with the Milford Haven boil-over data and assures CFD based multiphase modeling as an effective tool for predicting thermal hazards in petroleum storage systems.

Investigation of *Luffa Cylindrica* biochar as a performance enhancer in anaerobic digestion of organic waste

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Growing environmental problems and the limited supply of fossil fuels have increased the need of renewable energy sources. Anaerobic digestion is a promising technology for renewable energy generation and sustainable waste management, but its efficiency is slowed down by methane yield and unstable microbial activity. Biochar is a carbon-rich and porous material obtained through pyrolysis of biomass under limited oxygen condition and has gained attention as an additive to improve bio methanation process. In this study, biochar was prepared from luffa (*Luffa Cylindrica*) biomass, an unexplored agricultural byproduct with naturally fibrous and porous structure. The obtained biochar was comprehensively characterized using proximate and CHNS analysis, FT-IR, BET surface area measurement, XRD, ICP, pH and Zeta potential analysis. Six Laboratory scale digesters containing mixed food waste and fresh cow dung were designed to evaluate the role of luffa biochar in methane production. The results indicate that the biochar added setups produced more methane as compared to control digesters. The findings suggest that luffa biochar is an effective additive for improving the efficiency of anaerobic digestion, offering sustainable approach to optimize biogas production from organic waste while contributing to renewable energy development.

Circular Economy Approaches for Solid Waste Management: Innovations, Challenges, and Future Prospects

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Rapid urbanization, population growth, and evolving consumption patterns have escalated solid waste generation, posing environmental and health implications. Promoting circular economy (CE) principles has gained momentum as an effective, sustainable waste management strategy. The circular economy is based on four integrated terms described as the 4Rs: reduce, reuse, recycle, and recover. The CE's fundamental principles are industrial symbiosis, extended producer responsibility (EPR), and waste-to-energy (WTE) technologies. This review highlights successful case studies from nations like the Netherlands, Sweden, and India that can generate employment opportunities, encourage innovation, and create new business models. Significant challenges such as high initial investment costs, regulatory inconsistencies, and consumer behaviour resistance are critically examined. There is a need to implement a national CE framework that prioritizes EPR, incentivizes advanced recycling facilities, and creates demand for secondary materials. Additionally, the informal sector's role and public awareness initiatives must be encouraged to promote adequate source segregation and participation. The circular economy helps to achieve the Sustainable Development Goals (SDGs) by conserving resources, reducing waste, and promoting sustainable production and consumption

DFT Study of CO₂ Activation on Pristine and Functionalized V₂C MXene

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MXenes, a series of two-dimensional transition metal carbides and nitrides, have been of significant interest as promising materials for CO₂ capture and conversion due to their high conductivity and surface chemistry tunability. In this work, we investigate V₂C MXene using density functional theory (DFT) calculations to explore its suitability for CO₂ adsorption and activation. We studied the adsorption energy to understand the material's affinity for CO₂, as well as electronic properties such as the density of states (DOS) and charge transfer processes to study the dynamics of interaction. We also studied the effect of surface functionalization (like O, F, Cl, S, OH) on the efficiency of CO₂ capture to determine changes that can increase adsorption capacity. From our findings, we found that functionalization significantly affects the adsorption energy and electronic structure, thereby affecting the potential for CO₂ activation. Specifically, OH-terminated V₂C showed bending of CO₂ and formation of *COOH, which is a key intermediate in the CO₂RR. This research provides significant insights into the design of MXene-based materials for efficient CO₂ capture and conversion applications.

Chemical Modification of Used Cooking Oil and Brassica Carinata Oil for the Synthesis of Biolubricants via Epoxidation Reaction: A Sustainable Pathway for Bio-Based Alternatives

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The trend of using non-edible vegetable oils as a potential feedstock for lubricants is increasing day by day due to environmental concerns and fossil fuel depletion. This study examines the potentially sustainable alternatives, i.e., used cooking oil and Brassica carinata, non-edible oils in the lubricant industry, by examining their ability and efficiency in the production of biolubricants via the epoxidation method. In this work, firstly, the Fatty acid methyl esters of used cooking oil and Brassica carinata oil were produced from the CSIR-IIP patented method. These fatty acid methyl esters then undergo an epoxidation reaction followed by the ring-opening reaction of the epoxide formed in the presence of an acid catalyst. The highest yield of 90.0% was obtained. The Fatty acid methyl esters profile of the oils was determined using GC-FID. The synthesised product was confirmed using FTIR and NMR spectroscopy. In FTIR spectroscopy, the peak around 847 cm⁻¹ corresponds to the epoxy group, and the disappearance of this peak in the final product confirms the successful opening of the epoxide ring. The thermal stability of the biolubricants was examined using the TGA technique. The physicochemical properties of the products, including a density of around 0.9824 g/cm³ at 15°C, and a pour point of less than -10°C, are well comparable to those of ISO VG 10.

A new approach for Carbon Dioxide Sequestration and Utilization for Methane Recovery from Natural Hydrate-bearing Sediments

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Gas hydrates (GHs) are solid, ice-like crystalline materials formed by the encapsulation of natural gas (primarily methane) inside the cages of water molecules at suitable pressure and temperature conditions. GHs are considered a vast potential unconventional energy source for the future, as the amount of natural gas contained in these deposits globally is enormous, estimated to be between 100,000 and 300,000 trillion cubic feet, possibly surpassing all conventional natural gas reserves. However, there are significant technical challenges to overcome in order to safely and efficiently extract this untapped energy. These challenges include locating potential deposits, developing effective production methods, and managing geological hazards associated with extraction.

Herein, we are exploring a new approach to methane (CH₄) production that provides economic benefits through gas recovery and environmental advantages by reducing carbon dioxide (CO₂) emissions. This method also maintains reservoir stability by forming more stable CO₂ hydrates inside the porous sediments. A new high-pressure reactor facility, designed to replicate hydrate reservoir conditions, has been established at the upstream lab of CSIR-IIP. Arabian Sea sediments were used to create methane hydrate, which mimics natural hydrate-bearing sediments. CO₂ was injected into the methane hydrate bearing sediment at various temperatures ranging from 1-to-10 °C, and methane recovery was measured using gas chromatography. We also examined the impact of various additives, such as the surfactant sodium dodecyl sulfate (SDS), an in-house produced biosurfactant (Rhamnolipid), and the amino acid L-Tryptophan, on the kinetics of hydrate formation and dissociation (gas recovery). The methane hydrate saturation of the sediment ranged from 25% to 30%.

The addition of these additives improved methane recovery slightly, achieving a gas recovery of 40% to 45% within approximately 24 hours at a sediment temperature of around 3 °C, along with CO₂ storage of 15% to 25%. This integrated strategy for CH₄ recovery combined with CO₂ sequestration offers a promising pathway toward cleaner energy production and climate change mitigation.

Engineering $\text{Zn}_{12}\text{O}_{12}$ Nanocluster *via* Vacancies and Industrial Catalyst-Inspired Cu-Al Co-doping for CO_2 Conversion

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Electrochemical conversion of CO_2 to value-added fuels is widely recognized as a promising strategy for achieving carbon neutrality and renewable energy utilization. Yet, its industrial implementation is constrained by high power consumption and insufficient product selectivity. The industrial catalyst $\text{Cu}/\text{ZnO}/\text{Al}_2\text{O}_3$ is widely utilized for methanol formation, where ZnO plays a crucial role in CO_2 adsorption and intermediate stabilization during the hydrogenation steps. At the nanoscale, the $\text{Zn}_{12}\text{O}_{12}$ nanocluster serves as a unique model due to its tunable electronic structure, high surface area-to-volume ratio, and abundance of more uncoordinated sites, thereby making it particularly suitable for probing catalytic mechanistic studies. In this study, inspired by industrial catalyst, density functional theory (DFT) calculations were utilized to evaluate the influence of Cu, Al, Cu-Al doping, and vacancy engineering in $\text{Zn}_{12}\text{O}_{12}$ for CO_2 adsorption and its reduction mechanism to formic acid (HCOOH). Moreover, the competitive reactions, such as CO generation, are also taken into consideration over pristine $\text{Zn}_{12}\text{O}_{12}$, vacancy-engineered, and doped $\text{Zn}_{12}\text{O}_{12}$. Using HCOOH as a representative product as well as a probe for investigating the underlying mechanism, we find that Cu-Al introduction provides moderate performance for both CO_2 activation and intermediate stabilization, while vacancy engineering substantially improves CO_2 activation along with effective stabilization of formate (HCOO^*) and carboxylate ($^*\text{COOH}$) intermediates. Also, the key finding demonstrates that introducing Zn vacancy in $\text{Zn}_{12}\text{O}_{12}$ enhances the CO_2 adsorption compared to doped $\text{Zn}_{12}\text{O}_{12}$ systems. Furthermore, the comprehensive electronic analysis, including projected density of states (PDOS) and Bader charge analysis, reveals that improved interaction between CO_2 and the nanocluster is responsible for the enhanced activity and selectivity. Collectively, these findings demonstrate that defect engineering is a more effective strategy than doping for tuning $\text{Zn}_{12}\text{O}_{12}$ nanoclusters in CO_2 reduction.

Enhancing Walkability Through Green Infrastructure: A Perception-Based Study of Pedestrian Environments in Dehradun

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Walkability is central to sustainable and green urban development, due to its inherent characteristics such as contributing to active transportation, reduced dependency on vehicles, and thus reducing congestion and pollution. Previous studies identified that in order to promote safe and conducive walk environment, as proposed in several action plans and schemes such as SMART Cities, AMRUT, JnNURM, etc., it becomes important to pay due attention to rational planning of pedestrian facilities. However, rapid increase in motorization has marginalized pedestrians, resulting in unsafe environments and high fatality rates. In Dehradun, India, pedestrians remain the most neglected of the transportation sector, with issues including narrow or obstructed footpaths, unsafe crossings, and widespread encroachments. In order to dive to the root of this issue, a road-user perception-based study was conducted in the city, based on various dimensions of walkability, such as accessibility, comfort, and safety, walking willingness, built-environment, etc. The data was analyzed for inter-correlations among the various dimensions, through a dimension reduction framework such as Exploratory Factor Analysis (EFA). The EFA resulted in a set of key-indicators of walkability, which may be used as policy variable for promoting and developing pedestrian centric infrastructure development in Dehradun City.

Mg-MOF-74 Based Composite for Slow Release Fertilizer: An Approach Towards Greener Agriculture

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Due to increasing population and land dwindling, the pressure on agriculture has increased for productive growth and sustainable use of environment. This research introduces an approach for sustainable and eco-friendly slow release fertilizer (SRF) using a blend of metal organic framework (MOF), fertilizer, polymer, and activated sand. By using the high porosity and surface area of Mg-MOF-74, synthesized via solvothermal method, fertilizer was loaded into the MOF. Polymer was incorporated to ensure uniform polymer distribution, while activated sand provided structural integrity and controlled nutrient release. The composite was characterized using fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), surface area analyzer and X-ray photoelectron spectroscopy (XPS) and field emission scanning electron microscopy (FESEM), it shows needle shape of the MOF and uniform coating of the composite and confirms the successfully formed system. This work explores an efficient composite with improved nutrient utilization to reduces environmental impact. Employing Mg-MOF-74, fertilizer, polymer, and activated sand, an innovative method for SRF which aims sustainable agriculture. The results highlight the potential of the material in fertilizer technology, offers sustainable solution for agricultural demands of the society.

Sorption of Selenium Using Immobilized *Bacillus selenatarsenatis* 9470^T on Iron-Modified Dolochar: Box-Behnken Design and Machine Learning Approach

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The study immobilised *Bacillus selenatarsenatis* 9470^T on iron-modified dolochar (FeDBac) for selenium removal from aqueous solutions. The adsorbent was characterised using SEM, EDS, XRD, FTIR, pH_{zpc}, and BET analyses. The pH_{zpc} of FeDBac was found to be 8.3, a surface area of 17.8 m²/g, and an average pore diameter of 4.7 nm. Batch experiments designed via the Box–Behnken Design examined the effects of pH, dosage, and contact time, achieving maximum Se removal at pH 2, 10 g/L dosage, and 1.5 h contact time. Adsorption followed the Freundlich isotherm and pseudo-second-order kinetics, while thermodynamic analysis confirmed a spontaneous, exothermic process with low randomness. Competing ion studies revealed phosphate caused the greatest inhibition, followed by sulfate, nitrate, manganese, aluminium, zinc, and iron. Gaussian Process Regression accurately modelled the adsorption behaviour ($R^2 = 0.99$, RMSE = 0.484), validating its consistency with experimental results.

Fluoride Removal in Mine Water using Iron-modified Zeolite Prepared from Blast Furnace Slag

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Fluoride-rich mine water has a significant impact on both ecological and human health, necessitating low-cost and environmentally friendly solutions. This study develops an iron-modified zeolite synthesized from blast furnace slag (BFS) to remove fluoride efficiently from coal mine water. BFS was alkali-activated and hydrothermally crystallized to zeolitic phases, then functionalized with Fe(III) to create fluoride-affinitive surface hydroxyls. Material characteristics (XRD, FTIR, BET, FESEM/EDS, pH_{PZC}) confirmed crystalline zeolite formation and iron dispersion. A batch study was conducted to evaluate the effects of pH, dosage, contact time, initial concentration, and competing anions and cations on fluoride removal from both synthetic and real mine waste samples. Kinetic, isotherm, and thermodynamic analyses were used to determine the adsorption mechanism. Mechanistically, fluoride removal proceeds via inner-sphere complexation to Fe–OH sites, ion exchange within the zeolitic framework, and co-precipitation with iron (hydr)oxides. The maximum removal was found to be between 60% and 70% at different experimental conditions. Utilization of iron-modified zeolite derived from blast-furnace slag offers a low-cost, sustainable alternative adsorbent for fluoride ion removal from mine water.

Utilization of Industrial By-products in Alkali Activated Pavement Blocks as a Green Alternative to Cement

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The growing global emphasis on sustainability has accelerated the search for low-carbon and eco-friendly alternatives to conventional cement based construction materials. Although Ordinary Portland Cement (OPC) remains the most widely used binder, its high carbon footprint underscores the need for greener substitutes. This study investigates the development of high performance, cement-free pavement blocks through alkali activation of industrial by-products such as fly ash and ground granulated blast furnace slag (GGBS). Various mixtures were produced by partially or fully replacing OPC with GGBS (0%, 5%, 10%, 15%, and 100%), activated using sodium hydroxide (NaOH) and sodium silicate (Na₂SiO₃). The optimal slag mix was subsequently modified with fly ash to enhance the binder system. Mechanical and physical properties including density, water absorption, durability, and unconfined compressive strength were evaluated after 7, 14, and 28 days of curing. Microstructural and phase analyses were conducted using XRD, XRF, and FESEM. The alkali-activated fly ash and slag systems demonstrated significant strength gain, reduced porosity, and enhanced water resistance, achieving compressive strengths comparable to standard pavement blocks. The findings highlight the potential of alkali-activated binders as sustainable, durable alternatives to conventional cement, promoting circular economy practices and reducing the carbon footprint of the construction industry.

Green Synthesis and Comprehensive Characterization of *Cinnamomum tamala* Essential Oil Nanoparticles

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A sustainable method was used to synthesize and thoroughly characterize *Cinnamomum tamala* essential oil loaded nanoparticles. Incorporates Zn nanoparticles (ZnNPs) to improve stability and effectiveness. Using Fourier transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), and X-ray diffraction (XRD), structural and morphology characterization were performed.

The chemical interaction *C.tamala* EO bioactive elements and nanoparticle matrix FTIR shows effective encapsulation, SEM shows well distributed nanoscale well distributed particle size and XRD verified the crystalline nature and phase purity. Because the volatile components were shielded from deterioration, biological evaluation revealed that the encapsulated CEO had a significantly higher capacity in free radical scavenging tests than unencapsulated oil. Antimicrobial research demonstrates that pathogenic bacterial strains were superiorly inhibited and that encapsulation efficiency was positively connected with activity. These results demonstrate that CEO NPs are a natural nanopatform that may be used in pharmaceuticals, therapeutic delivery system, antibacterial and antioxidant agents.

Fatigue behavior of Sustainable Low-Carbon micro alloyed Dual-Phase Steel for Next-Generation Automotive Components

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Pursuing sustainable and energy-efficient materials for automotive applications has increased due to the global drive toward decarbonization. Low-carbon micro-alloyed dual-phase (DP) steels offer a cost-effective and recyclable alternative to high-alloy advanced high-strength steels (HAG-AHSS). Their lower alloying content, better weldability, and simplified processing routes reduce production costs and energy consumption, improving resource efficiency and sustainable material utilization. In this study, a 0.05 wt.% C micro-alloyed ferrite–martensite DP steel sheet with superior mechanical performance was developed through advanced thermomechanical processing and controlled phase transformation. High-cycle fatigue (HCF) behavior was investigated at 520, 550, and 580 MPa stress amplitudes to evaluate its cyclic durability under automotive loading conditions. Microstructural evolution during fatigue was characterized using electron backscatter diffraction (EBSD) in a field-emission scanning electron microscope (FESEM). The findings reveal that the developed DP steel exhibits excellent fatigue resistance comparable to HAG-AHSS. It offers enhanced recyclability, reduced energy input, and a lower environmental footprint, making it a promising sustainable solution for next-generation automotive structures.

Modern Strategies towards Green and Sustainable Synthesis of Macrocyclic Assemblies

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Many pharmaceutical chemicals and bioactive natural substances have macrocyclic scaffolds. Numerous aza-macrocyclic compounds have been identified and produced for their drug-like properties and therapeutic values. Synthesis of these macrocyclic compounds is one of the most strategic steps in the production of a novel macrocycle. Over the past few decades, tremendous progress has been achieved in the field of total synthesis of macrocycles. To overcome traditional complicated procedures and excessive use of corrosive acids and toxic solvents, newer, uncomplicated, cost-effective and environmentally friendly methods have been developed. Frequently employed synthetic approaches are ring-closing mechanisms, click reactions, metal-catalysed cross-coupling, macrolactonization and macrolactamization. Furthermore, the use of high-concentration methods, green catalysts, solvent-free synthesis, solid-phase synthesis, and the use of green solvents like PEG-200 are offering an economically advantageous methodology for the synthesis of macrocycles. Hopefully, this review will be informative for researchers to establish a sustainable and effective synthesis methodology for designing novel macrocyclic complexes.

Comparative Adsorption Isotherm Analysis of Rose Bengal Dye on Gold-Decorated and Unmodified Activated Carbon

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In this study, activated carbon modified with gold nanoparticles (AC-GNP) was prepared by mechanically blending a GNP suspension with activated carbon in an agate mortar to improve its adsorption and degradation performance toward Rose Bengal dye. Surface characterisation using BET analysis confirmed that gold incorporation improved surface properties, increasing BET surface area from 13.027 m²/g for AC to 16.844 m²/g for AC-GNP, suggesting the availability of additional active adsorption sites. The adsorption performance of AC and AC-GNP was systematically evaluated by treating RB dye solutions with concentrations ranging from 10 to 50 ppm using 20 mg of adsorbent, while degradation was monitored using UV–vis spectrophotometry at 548 nm. The AC-GNP composite exhibited superior efficiency, achieving 97% degradation of 50 ppm RB dye compared to 52% using AC under identical conditions. Isothermal modelling revealed that both adsorbents followed the Langmuir model with high correlation coefficients ($R^2 > 0.92$), demonstrating monolayer adsorption. The maximum adsorption capacities (q_{\max}) were calculated as 52 mg/g for AC and 23.2 mg/g for AC-GNP composite, indicating strong affinity in the initial concentration range tested. The synergistic effect of GNPs with AC enhances adsorption and catalytic degradation, making AC-GNP highly effective for dye wastewater treatment.

Quantitative Variation of Shikimic Acid in Needles of *Pinus roxburghii*

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Pinus roxburghii, a dominant conifer of the Himalayan region, is often viewed as a contributor to forest fires due to its abundant and highly inflammable needle litter. It is also considered invasive for its rapid spread at the expense of native vegetation. Nevertheless, the species plays a vital ecological role by serving as a significant carbon sink in challenging mountainous terrains and by releasing atmospheric terpenes that enhance air quality and environmental resilience.

The present study investigates the potential of *P. roxburghii* needles as a renewable source of shikimic acid, a key precursor for the antiviral drug Oseltamivir (Tamiflu) currently derived mainly from imported *Illicium verum* (Chinese star anise). High-performance liquid chromatography (HPLC) analysis revealed shikimic acid contents ranging from 2.5–3.7% in tender needles, 2.34–2.59% in young needles, and 1.5–1.84% in mature needles. The observed decline with needle maturation suggests its metabolic conversion into aromatic amino acids such as tryptophan, tyrosine, and phenylalanine. The study elaborated on the variation of shikimic acid and its transformation to other compounds at different stages of maturity, which provides a useful baseline for further biochemical investigations.

Green Lungs of the City: Assessing Carbon Sequestration and Storage Potential of Urban Tree Species in Indian Capital

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Urban trees play an important role in mitigating climate change through capturing and storing atmospheric carbon dioxide within their biomass. This study assesses the carbon sequestration and storage potential of selected tree species planted in urban ecosystems of New Delhi, including *Azadirachta indica* (Neem), *Ficus religiosa* (Peepal), *Delonix regia* (Gulmohar), *Albizia saman* (Rain Tree), and *Cassia fistula* (Amaltas). Using field-based biomass estimation and a dynamic growth model (CO₂FIX), both aboveground and belowground carbon pools were quantified across representative urban sites. Results indicate that *Ficus religiosa* and *Azadirachta indica* exhibit the highest carbon accumulation potential, which is linked to their larger canopy spread and higher biomass density. This study also emphasized that bioenergy and carbon sequestration may be the best ways to mitigate CO₂ emission while addressing the climate change. The findings underscore the importance of species selection and management in enhancing urban carbon sinks and fostering climate-resilient cities. Integrating urban forestry into climate policies can strengthen India's pathway toward sustainable urban development and fulfilment of various Sustainable Development Goals (SDGs).

Development of Potential Flame Retardant to Enhance Cotton Safety

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The present study focuses on the development of a promising flame retardant finish for cotton fabric using a PNH-based system. Cotton, which is a highly flammable material having cellulose-based system, requires efficient flame retardant treatments to enhance its thermal stability and fire safety performance in design interiors, home textiles and industrial settings. In this work, a PNH formulation was synthesized and applied to cotton fabric through a pad-dry-cure technique under optimized conditions with different composition of chemicals. The treated samples were evaluated for limiting oxygen index (LOI), vertical flame test (VFT), to assess their flame retardant efficiency. The PNH-treated fabric shows a significant increase in LOI value compared to the untreated cotton, indicating improvement in flame resistance. Elemental analyses confirmed the presence of phosphorus and nitrogen on the fabric surface, which contributed to the formation of a protective char layer during combustion. This char acts as a barrier, limiting heat transfer and reducing the release of volatile flammable gases. Furthermore, the treated fabric maintained acceptable tensile strength and washing durability, demonstrating the potential of the PNH system as an efficient flame retardant for textile applications. Overall, the study establishes PNH as a promising alternative to conventional halogenated flame retardants, combining high performance with environmental safety.

Nitrogen Functionalized Schiff Base Biochar Hybrids as Dual Adsorbentsf Heavy Metal Remediation and CO₂ Capture

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Schiff base metal complexes, with their structural versatility and strong coordination affinity, offer an advanced platform for selective metal sequestration. In this work, pyridine- and pyrrolidine-based Schiff base complexes were synthesized and immobilized on lotus seedpod biochar produced at 500 °C and 800 °C, enabling a comparative evaluation of their adsorption efficiency and kinetic behaviour. Batch experiments were conducted across pH 3.0, 7.0, and 12.0, contact times of 0, 5, 10, 20, 30, 60, 120 min, and temperatures of 25 °C and 45 °C. The pyrrolidine-derived composites consistently outperformed their pyridine analogues, achieving 96.2 % Pb²⁺ and 93.1 % Cd²⁺ removal at pH 7 and 45 °C within 60 min. Kinetic fitting indicated pseudo-second-order behaviour ($R^2 > 0.99$). The superior activity of pyrrolidine complexes was attributed to, stronger σ -donation from the –NH and –CH₂ groups, enhancing coordination and electrostatic interactions with metal ions. The 800 °C biochar matrix exhibited greater porosity and surface basicity, reflected in higher CO₂ adsorption (3.4 mmol g⁻¹) compared to the 500 °C variant (2.6 mmol g⁻¹). Collectively, these results underscore the synergistic effect of nitrogen-rich pyrrolidine ligands and high-temperature biochar support in driving rapid, efficient, and thermally robust adsorption processes for heavy metal and CO₂ remediation.

Sustainable Nanofibrous Air Filters: Synergistic Performance of Biochar and TiO_2 within a Cellulose Acetate Matrix

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Airborne particulate matter ($\text{PM}_{2.5}$ and PM_{10}) continues to present serious threats to both human health and the environment, underscoring the need for sustainable and high-efficiency filtration materials. In this study, three types of electrospun cellulose acetate (CA) nanofibrous membranes were developed for air filtration: (i) CA-biochar, (ii) CA- TiO_2 , and (iii) a layered CA-biochar- TiO_2 composite in which biochar and TiO_2 were co-deposited between two CA nanofibre layers. The biochar, derived from poultry litter pyrolyzed at 500 °C, exhibited a highly microporous carbon framework enriched with oxygen-containing surface groups. Optimized electrospinning parameters yielded uniform fibres with an average diameter of 460 ± 45 nm and a porosity of 83%. Incorporating biochar and TiO_2 enhanced the membrane's surface roughness, specific surface area, and functional performance without compromising flexibility or biodegradability. The CA-biochar membrane displayed a high CO_2 adsorption capacity of 438 mg g⁻¹ owing to its microporous nature, while the CA- TiO_2 membrane demonstrated excellent photocatalytic and antibacterial properties under UV illumination. The layered CA-biochar- TiO_2 composite showed the best overall performance, achieving 95.4% removal of $\text{PM}_{2.5}$ and 99.2% of PM_{10} at a face velocity of 0.8 m s⁻¹, with a low pressure drop of 63 Pa. Additionally, its mechanical strength improved by 35% compared to pure CA membranes, and thermal stability remained consistent up to 315 °C. These results emphasize the synergistic interactions between biochar and TiO_2 within the biodegradable CA matrix, offering a sustainable pathway toward multifunctional air filters capable of efficiently removing particulate, gaseous, and microbial pollutants.

Life Cycle Assessment of Municipal Solid Waste Management: Comparative Evaluation of Existing Technologies in India

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Solid waste management is a very challenging task, especially for developing and higher population countries like India. Since the treatment method of solid waste involves various techniques, which may be responsible for various environmental emissions. The present study explore a comparative Life Cycle Assessment (LCA) of municipal solid waste (MSW) management strategies including landfilling, composting, anaerobic digestion (AD), and torrefaction, with emphasis on environmental burdens, energy recovery potential, and implications for policy in Indian urban contexts. For this SPHERA (or GaBi) was used to evaluate multiple scenarios representative of contemporary urban practice and proposed alternatives that significantly reduce the emissions. Results show that biological treatment routes (composting and AD) consistently yield lower global warming potential (GWP) and reduced acidification and ecotoxicity impact relative to unmanaged landfilling. Torrefaction of organic residues demonstrates potential for producing higher-energy solid fuels and reducing moisture-related transport burdens, but its net benefits depend strongly on feedstock and process energy demand. This study recommends prioritising composting and AD at scale, coupled with improved segregation and policy incentives as practicable pathways to lower environmental burdens in Indian MSW systems.

Luminescent Sensing of Biogenic Phosphates via Imidazo-Phenanthroline Functionalized Ruthenium(II) Probe

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Ru(II)-polypyridyl complex Ru-Q1, incorporating anion-recognition sites, was synthesised and comprehensively examined for its anion sensing performance. Among a range of tested species, the probe Ru-Q1 displayed remarkable selectivity and sensitivity toward the biogenic phosphate ions (H_2PO_4^- and $\text{HP}_2\text{O}_7^{3-}$), evidenced by significant luminescence quenching accompanied by red-shifted emission. Fluorescence titration experiments yielded detection limits of 0.813 μM for H_2PO_4^- and 0.6 μM for $\text{HP}_2\text{O}_7^{3-}$, with corresponding binding constants of $8.5 \times 10^4 \text{ M}^{-1}$ and $4.5 \times 10^5 \text{ M}^{-1}$. Competitive ion studies further validated the probe's high selectivity, maintaining its response even in the presence of other metal ions. Mechanistic understanding was supported by Job's plot analysis, ^1H NMR titrations, FE-SEM imaging, emission lifetime measurements, and DFT studies. The possible binding/packing geometry of the phosphate with the probe was further supported by EDAX and FT-IR analysis. Moreover, cellular imaging in HepG2 cells confirmed its biocompatibility and potential utility in biological environments.

Mechanistic Divergence in Hydrogen Bonding: Catechol Based Recognition of Cyanide and Fluoride

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Catechol-derived Schiff bases offer a versatile framework for anion sensing, where intramolecular hydrogen bonding plays a decisive role in modulating selectivity and emission behavior. In this work, we present PyCt, a catechol based fluorescent probe capable of discriminating cyanide (CN⁻) and fluoride (F⁻) through mechanistically distinct interactions. Spectroscopic analyses reveal that CN⁻ engages the phenolic –OH via hydrogen bonding without full deprotonation, whereas F⁻ induces complete deprotonation, disrupting the native hydrogen bonding network. These contrasting modes yield selective fluorescence turn-on responses at 535 nm (CN⁻) and 544 nm (F⁻), driven by enhanced intramolecular charge transfer (ICT) and excited-state stabilization. Binding stoichiometry was confirmed as 1:1 through Job's plot, ¹H NMR titration, and DFT calculations. PyCt demonstrates high sensitivity (LoD: 0.42 μM for CN⁻; 1.20 μM for F⁻), excellent selectivity, and reversible recognition. Real-sample validation in food matrices (apple seeds, bitter almonds, kidney beans) and smartphone-assisted RGB quantification underscore its practical utility for portable anion detection. These findings highlight PyCt's potential for real-world sensing applications and mechanistic exploration of hydrogen-bonding-driven selectivity.

Compostable Plastics: A Sustainable Solution or the Next Environmental Myth?

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With the increasing concerns over plastic pollution have been driving a global shift towards compostable plastics. Materials such as Polylactic acid (PLA), polyhydroxyalkanoates (PHA), and polybutylene adipate terephthalate (PBAT) and starch blends are claimed to biodegrade within 90 days under industrial composting conditions. But evidence suggests incomplete degradation, leaving behind microplastics fragments and undecomposed additives that pose ecological and toxicological risks. The incorporation of undisclosed plasticizers, stabilizers, colorants, and compatibilizers, some of which are known as endocrine disrupter and a persistent organic pollutant raises additional questions about their environmental safety. These additives may also inhibit microbial activity besides deteriorating the compost quality. The irony of compostable plastics will be discussed critically in the current paper, though intended to replace the traditional plastics, still the complexity of their chemical composition and low degradation may create new pollution pathways. This study emphasizes the need to propose stronger additive disclosure rules, region specific biodegradation guidelines and testing frameworks to ensure compostable plastics truly support a circular and sustainable future.

Electrodeposition Optimization of Ni-Fe Electrode for Alkaline Water Splitting: Effect of Salt Ratio, Deposition Time and Deposition Potential Integrated with AI-Driven Performance Modeling

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Ni-Fe based electrocatalysts are widely recognized as promising non-noble-metal alternatives for efficient alkaline water electrolysis, owing to their synergistic catalytic activity toward both the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). However, their performance strongly depends on deposition parameters that govern alloy composition, morphology, and surface activity. In this study, we systematically investigate the influence of three key electrodeposition variables metal-ion ratio (Ni:Fe), applied deposition potential, and deposition time on the structural and electrocatalytic behaviour of Ni-Fe alloy films. A factorial design approach was employed to explore parameter interactions, enabling optimization with minimal experimental runs. The deposited electrodes were evaluated using Linear sweep voltammetry and Tafel analysis to quantify OER performance. Preliminary findings reveal that moderate Fe incorporation, optimal reduction potential near the transition region of hydrogen evolution, and controlled deposition time lead to enhanced catalytic activity and improved surface microstructure. This systematic investigation establishes a parameter performance correlation for Ni-Fe electrodes and provides a foundation for data-driven optimization and future machine-learning-assisted catalyst design for overall water splitting.

Enzymatic Treatment of Textile and Dye Waste: Degradation by Oxidoreductases

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The textile sector produces large amounts of wastewater that are contaminated with the dyes that are hazardous to human health and ecologies. Sustainable substitutes to traditional treatment processes are urgently needed as they are often expensive and lead to secondary pollutants. Enzymatic therapy has been very promising when oxidoreductases like laccases, manganese peroxidases, and lignin peroxidases are used as an environmentally-friendly solution. They are enzymes produced by fungus, bacteria, algae, plants, and extremophiles, are broad-substrate specific, with high catalytic potential, and are capable of breaking down complex dyes into less hazardous chemicals. Recent advances in enzyme engineering, immobilization and bioreactor design have made them more stable, reusable and industrially applicable. This chapter highlights the microbiological origin of ligninolytic enzymes, color degradation techniques, recent developments and the challenges associated with scaling up enzyme systems.

Comparative Analysis of Simulated and Actual Performance of Solar PV Systems

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Grid-connected solar PV systems play a vital role in decreasing the carbon emissions and fulfill the energy demands. Current research work investigates the performance of a 100kWp PV system using PVsyst simulation and real-time monitoring. The methodology comprises system modeling, data collection, and comparative analysis of predicted and actual energy generation. The outcomes show that the system attained a specific yield of 1427 kWh/kWp/year and a performance ratio (PR) of 82.6%, with major losses attributed to temperature (8%) and soiling (3%). The study highlights discrepancies between simulated and actual performance, underscoring the need for accurate environmental data and continuous monitoring. Recommendations include improved cleaning schedules and temperature management strategies to enhance efficiency. This work provides insights for optimizing PV system design and ensuring reliable energy output under varying climatic conditions.

Economics and Environmental Performance Analysis of Solar Water Pump Using PVsyst

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The current work evaluates the performance of a solar water pumping system using PVsyst software, focusing on energy output, cost savings, and environmental profits. The system was designed for a site with an average solar irradiation of 5.2kWh/m²/day and a static head of 18m. The PVsyst simulation predicts an annual energy generation of approximately 14,500kWh, sufficient to pump 109,000 m³ of water per year. Economic analysis shows a payback period of 5.2 years, with lifetime savings exceeding ₹2.8 lakh compared to diesel pumps. Environmental assessment indicates a reduction of 12.5 tons of CO₂ emissions annually. These results confirm that solar water pumps are cost-effective, reliable, and environmentally sustainable for agricultural applications.

Bioethanol Production from Lignocellulose Waste

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The urgent need for sustainable energy solutions has intensified the research into bioethanol production from lignocellulosic biomass and industrial waste. This study aims to investigate bioethanol production from lignocellulosic waste. In this study, we followed a three-step process for bioethanol production from lignocellulosic biomass. After treating the lignocellulosic biomass with alkali (sodium hydroxide), enzymatic hydrolysis was conducted to release fermentable sugars. Finally, the sugars were converted to ethanol using yeast *saccharomyces cerevisiae*. The extraction of ethanol was done using TBP (tri-n butyl phosphate) by solvent extraction process. The quantification of glucose and alcohol was carried out using UV-Vis spectroscopy via DNS and dichromate method respectively. The process showed 32% conversion to fermentable sugars showing good efficiency of process. These findings reinforce the suitability of lignocellulosic biomass for bioethanol production via enzymatic route. This presents a sustainable perspective addressing the issue of lignocellulosic waste and renewable energies generation. The study represents a promising and effective substrate for bioethanol production offering a practical pathway for transforming waste into renewable fuel.

Investigation of Microplastic Contamination in Human Exposure Pathways and its Toxic Effects

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Microplastics in the real environment have extremely complex sources with more diversified occurrences and more hidden hazards, which brings about great challenges in revealing their toxic effects and potential health hazards. In order to determine the risk of microplastics to human health, one of the main problems is the lack of information about microplastics to which humans are exposed. The qualitative and quantitative analysis methods of microplastics in the real environment limit the research on their source, occurrence, and toxicity. Microplastics are the silent killer which is present everywhere all over the globe. The minute size (ranging from 1micrometer to 5 millimeter), diverse chemical composition and strong adsorption capacity for toxic microplastics make them a growing concern for human health. Humans are exposed to microplastics daily via oral, inhalation, dermal pathways and through some medical procedures. It's found in human brain, placenta, urine, blood and bone marrow. It can cause oxidative stress, inflammation, endocrine disruption and DNA damage. Understanding the pathways and effect on human is crucial for developing mitigation of microplastics, choosing standardized analytical methodologies and protecting human and environmental health against rising threat of microplastics.

Extending the Carbon Backbone of Biorenewable Furaldehydes by Benzoin Condensation and the Synthesis of Novel 2,4,5-Trisubstituted Imidazoles

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Carbohydrate-derived furaldehydes are leading the biorefinery research as renewable platform chemicals for synthesizing organic chemicals. The derivatives of furfurals can be classified based on the number of carbon atoms in their skeletal system. Organic molecules possessing more carbon atoms in their molecular structure than furfurals involve a C–C bond-forming reaction as a key transformation during their synthesis. The transformations are preferably carried out under catalytic conditions to maximize the sustainability of the approach. In this regard, benzoin condensation is a well-documented C–C bond-forming reaction performed under catalytic conditions. N-Heterocyclic carbenes (NHCs) are used as green catalysts for the transformation under base catalysis. The functionalities in the benzoin product (e.g., ketone) can be exploited further to synthesize novel heterocyclics with potential applications as bioactive compounds. This study reports the benzoin condensation reaction of carbohydrate-derived furaldehydes through the conventional and microwave-assisted synthetic method using organic tertiary amines as bases and thiamine hydrochloride (Vitamin B1) as the NHC catalyst. The effect of various bases on the efficiency of the benzoin condensation reaction was explored under conventional heating and microwave irradiation (MWI). The ratio of furil and furoin product was successfully controlled by modifying the reaction conditions. Moreover, the renewable furoin/furil derivatives were transformed into novel 2,4,5-trisubstituted imidazoles under various acid catalysts. It was observed that MWI significantly accelerated the reaction kinetics for furoin formation. All the furoins and 2,4,5-trisubstituted imidazoles were obtained in good to excellent isolated yields under optimized conditions.

Transforming Plastic Waste into Liquid Fuels: Novel Upgrading of Polypropylene Pyrolysis Oil and Utilization in Diesel Engine

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The end-of-life polypropylene (EOL-PP) items have created serious environmental concerns due to the accumulation of slowly degrading polypropylene (PP) in landfill sites. Indiscriminate disposal of EOL-PP leads to pollution (air, water, and soil), posing health-, fire-, and ecological hazards. In this regard, pyrolysis of EOL-PP items into polypropylene pyrolysis oil (PPO) is a scalable, economically feasible, and environmentally acceptable waste management strategy. An inexpensive, scalable, and eco-friendly upgrading method for crude PPO (CPPO) is required for fuel use in engines owing to its poor stability (e.g., storage, oxidative) and inferior physicochemical properties. This work reports a novel upgrading of CPPO into upgraded PPO (UPPO) by sequentially removing the excessively volatile and chemically unstable components in a two-step process. The chemical composition of the volatile fraction (b.p. <150 °C) resembled gasoline and heavy naphtha fraction, which diversifies the applications and markets for PPO. The physicochemical properties and spectral characteristics of CPPO and UPPO were analyzed to quantify the improvements in fuel properties. The results showed that UPPO had noticeably better physicochemical properties than CPPO.

<i>Physicochemical Properties</i>	<i>ASTM Methods</i>	<i>Unit</i>	<i>Diesel</i>	<i>CPPO</i>	<i>UPPO</i>
Density at 15 °C	D4052-22	g/cc	0.831	0.799	0.812
Kinematic Viscosity at 40 °C	D7042-21a	cSt	2.781	2.126	3.385
Pour Point	D5950-14	°C	-6	-24	-9
Flash Point	D93-20	°C	47	<20	47.5
Sulfur Content	D7220-22	ppm	6	46.5	38
Acid Value	D664-24	mg KOH/g	0.06	5.82	0.54
Calorific Value	D240-19	MJ/kg	45.50	44.88	45.99

UPPO was then blended (10-25 vol%) with diesel and the fuel blends were used in a diesel engine to study the engine performance and emission characteristics. The UPPO-diesel blends showed comparable engine performance (e.g., BTE) and reduced emissions (i.e., NO_x, CO, and unburnt hydrocarbons) compared to unblended diesel.

Design and Development of a Solar Assisted Floating Drum Biogas Reactor for High Altitude Area

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Anaerobic digestion (AD) is an eco-friendly and sustainable technology for organic waste management, providing key benefits such as sludge reduction and renewable biogas production. Temperature critically affects the AD process and biogas yield, particularly in colder regions where low temperatures suppress microbial activity. For instance, cities in Uttarakhand, such as Dehradun and Uttarkashi, often experience significant drops in biogas production during winter due to the inactivation of methanogenic bacteria.

To address the challenge of reduced biogas output under cold climatic conditions, this study focuses on the development of a solar-heated, floating-drum biogas plant. A portable 1 m³ floating-drum biogas digester has been designed and integrated with a solar heater via heat exchangers to maintain optimal digester temperatures. The proposed system combines a floating drum type digester (LCTD) with a solar water heating system (SWHS) using a mild steel heat exchanger. This innovative setup minimizes heat loss and enhances heat transfer efficiency, offering dual heating modes for the digester: direct solar absorption during the day and SWHS-assisted heating at night. This approach aims to simultaneously improve waste management and biogas production in the cold regions of Uttarakhand.

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The background of the entire page is a complex, abstract molecular structure. It consists of numerous interconnected nodes, represented by circles of varying sizes and colors (red, teal, black, and light grey). These nodes are connected by thin, light grey lines, creating a dense, web-like pattern that resembles a chemical or biological network. The overall effect is a sophisticated, scientific aesthetic.

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