

First International Conference on

INNOVATIONS IN MATERIAL CHEMISTRY FOR SUSTAINABILITY



18-20

February 2026

Organized by

**DEPARTMENT OF CHEMISTRY &
CENTRE FOR MATERIAL CHEMISTRY**

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February 18-20, 2026

Editors

Dr. A. Thangamani Dr. K. Saravana Mani
Dr. A. Manikandan Dr. D. Manoj

Organized by



**Department of Chemistry &
Centre for Material Chemistry (CMC)
KARPAGAM ACADEMY OF HIGHER EDUCATION
Pollachi Main Road, Eachanari Post, Coimbatore – 641 021,
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Editors: Dr. A. Thangamani Dr. K. Saravana Mani, Dr. A. Manikandan and Dr. D. Manoj.

ABOUT THE INSTITUTION

Karpagam Academy of Higher Education (KAHE), a premier Deemed-to-be University, is committed to holistic learning and research excellence. The institution encompasses five faculties: Arts, Science, Commerce & Management; Engineering; Architecture, Design & Planning; Pharmacy; and Performing Arts.

It also hosts 13 specialized research centers that drive innovation, interdisciplinary collaboration, and pioneering research. KAHE has consistently been recognized for its academic and research achievements, securing a position in the 101-150 rank band in the NIRF University Rankings.

On the global front, it is ranked in the Times Higher Education 2025 Interdisciplinary Subject Rankings (401-500) and the Impact Rankings (401-600). With a strong research profile of over 7,500 publications, 70,000 citations, an institutional h-index of 96, and 147 granted patents, KAHE continues to expand knowledge, strengthen international collaborations, and affirm its position as a leading institution in higher education.

ABOUT THE DEPARTMENT

The Department is running Postgraduate (PG) and Ph.D. programs. The Department is equipped with sophisticated instruments like HPLC, UV-Visible Spectrometer, FT-IR Spectrometer, Gas Chromatographic analyzer, etc.

The main objective of the Department is to impart knowledge among the students in basic areas of Chemistry. Apart from the core courses, knowledge about the latest trends in Chemistry, including Green Chemistry, Medicinal Chemistry and Nanochemistry, is also included in the regular curriculum.

Department of Chemistry established two Centres of Excellences, namely, the Advanced Battery Research Centre (ABRC) and the Centre for Material Chemistry (CMC). ABRC is equipped with computer-controlled battery testers and offers test facilities as per International Standards such as IIS, EN, SAE and ICE.

ABOUT THE CENTRE FOR MATERIAL CHEMISTRY (CMC)

Centre for Material Chemistry (CMC) is well-established and one of the premium centre at KAHE. CMC is equipped with sophisticated equipment's like Fluorescence Spectrophotometer, TG-DA Thermal analyzer, DSC Thermal analyzer, UVDRS Spectrophotometer, FT-IR Spectrometer (ATR), and Electrochemical workstation.

Currently, the faculties at the centre are working in Electrochemical sensors, Photocatalysis, Supercapacitors, Fluorescent Organic Materials and Pigments.

ABOUT ICIMCS – 2026

The International Conference on Innovations in Material Chemistry for Sustainability (ICIMCS-2026) aims to provide a common platform for knowledge sharing among Researchers, Academicians, Practitioners, and Industrialists in areas related to Chemistry and Sustainable Technologies.

It provides a forum for discussing the most recent innovations, trends, experiences and concerns. It will also stimulate efforts to integrate the latest approaches to strengthen and help in shaping its future by fostering communication among participants. The conference will also include keynote addresses by renowned Academicians, Scientists, and Industrialists from Leading organizations, oral and poster presentations.

The Conference will provide the authors and listeners with opportunities for National and International collaboration and networking among Institutions from India and abroad for promoting research and developing Sustainable Technologies.

CONFERENCE THEME (RESEARCH AREAS)

Sustainable Materials and Technologies
Synthetic Organic Chemistry
Fluorescent Organic Materials
Catalysis
Fuel Cells
Electrochemical Corrosion and Surface Protection
Energy Conversions and Batteries
Nano Composites for Biological Applications
Supramolecular Chemistry
Electrochemical Sensors
Green and Environmental Chemistry
Polymer and Industrial Chemistry
Quantum Chemistry and Technologies
Chemical and Bio-sensors
Bioinorganic Chemistry
Computational Chemistry

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MESSAGE FROM THE PRESIDENT



Dr. R. Vasanthakumar
President

It is with great pleasure that I extend my warmest greeting and congratulations on the successful organization of the first International Conference on “Innovations in Material Chemistry for Sustainability (ICIMCS-2026)” by Department of Chemistry & Centre for Material Chemistry, Karpagam Academy of Higher Education.

In our pursuit of excellence, we recognize that the most meaningful research is the one which directly addresses the planet’s pressing challenges. The major theme of ICIMCS-2026 is therefore profoundly timely, focusing on the development of sustainable materials and techniques for environment, energy and health.

I sincerely appreciate the high caliber of the research presented by the renowned national and international speakers, faculties, and research scholars. May this conference spark new ideas, foster enduring global collaboration, and ultimately, pave the way for translational breakthrough that truly benefit humanity,

I look forward to the significant accomplishments that will emerge from the knowledge shared within these proceedings.

President
Karpagam Academy of Higher Education

MESSAGE FROM CHANCELLOR



**Prof. Dr. K. Ramasamy,
Chancellor**

I am extremely delighted to know that the Department of Chemistry & Centre for Material Chemistry, Faculty of Arts, Science, Commerce and Management, Karpagam Academy of Higher Education are organizing the first International Conference on “Innovations in Material Chemistry for Sustainability (ICIMCS-2026)” from February 18 to 20, 2026.

Chemistry continues to be a driving force behind many of today’s innovations. Recent advancements in Materials Chemistry have led to significant breakthroughs that are revolutionizing how we approach both everyday problems and complex global issues.

The major research themes of ICIMCS-2026 are Sustainable Materials and Technologies, Energy Conversions and Batteries, Green and Environmental Chemistry and Synthetic Organic Chemistry. I am sure that the research topics which are going to be discussed in the conference will certainly bring an opportunity for deliberations on the latest advancements in Materials Chemistry and sustainability. I hope the ideas and discussions which emerged from ICIMCS-2026 will lead to spin-off benefits to academia and industries.

I wish the conference a grand success.

**Chancellor
Karpagam Academy of Higher Education**

MESSAGE FROM VICE-CHANCELLOR



**Prof. Dr. S. Ravi,
Vice-Chancellor**

I am extremely delighted to note that the Department of Chemistry & Centre for Material Chemistry, Faculty of Arts, Science, Commerce and Management, Karpagam Academy of Higher Education are organizing Anusandhan National Research Foundation (ANRF) sponsored International Conference on “Innovations in Material Chemistry for Sustainability (ICIMCS-2026)” from 18th February to 20th February, 2026.

The advancements in Materials Chemistry have led to innovations in sustainability. The innovations in sustainable Chemistry mitigates environmental and economic challenges and foster a healthier earth for future generations. Hence, I am sure that the major theme of this conference is significant and it would be beneficial to researchers, and students. It will also inculcate the research culture among the entire fraternity of Education in the country, thereby, contributing to the nation's development.

I hope that this conference will certainly induce innovative ideas among the participants, paving the way for new inventions and technologies in various aspects of sustainable Chemistry. I congratulate the organizing team for conducting ICIMCS-2026 in our esteemed University.

I wish the conference a grand success.

**Vice-Chancellor
Karpagam Academy of Higher Education**

MESSAGE FROM THE REGISTRAR



**Prof. Dr. B. V. Pradeep,
Registrar**

I am extremely happy to note that Department of Chemistry & Centre for Material Chemistry, Faculty of Arts, Science, Commerce and Management, Karpagam Academy of Higher Education are organizing an International Conference on “Innovations in Material Chemistry for Sustainability (ICIMCS-2026)” on 18th to 20th February, 2026 and it is sponsored by Anusandhan National Research Foundation (ANRF), Government of India.

The scientific research on materials chemistry is conducted in academic institutions, research centers, and industries. The positive research outcomes from the fruitful scientific research play a critical role in improving the standard of living as well as providing sustainable solutions for various global issues. The sharing of results and information from the research that are related to sustainable Material Chemistry is required among the researchers and students. Certainly, ICIMCS-2026 would be a great platform to share and discuss the current innovations from the Sustainable Chemistry.

I congratulate the convenors and the team for conducting such an important conference in our esteemed University.

My hearty wishes and grand success of the conference.

**Registrar
Karpagam Academy of Higher Education**



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Prof. Dr. S. VINCENT, D.Sc., FNABS., FASCh., FRSB (Lon),
Member Secretary



MESSAGE

It gives me immense pleasure to extend my warm greetings on the occasion of the ANRF sponsored 1st International Conference on *Innovations in Material Chemistry for Sustainability (ICIMCS-2026)* organized by the Centre for Material Chemistry, Department of Chemistry, Karpagam Academy of Higher Education, Coimbatore.

The theme of ICIMCS-2026 is both timely and vital. In the present global context, innovations in material chemistry play a transformative role in addressing pressing challenges related to energy, environment, climate change, resource efficiency, and sustainable development. This conference provides a dynamic platform for researchers, academicians, industry experts, and young scholars to exchange ideas, present cutting-edge research, and explore interdisciplinary collaborations that drive sustainable technological progress.

I commend the organizing committee for their dedicated efforts in bringing together distinguished speakers and participants from across the globe. I am confident that ICIMCS-2026 will inspire meaningful discussions, foster new partnerships, and contribute significantly to the advancement of sustainable material science research. I wish the conference great success.

With best wishes,


MEMBER SECRETARY

MESSAGE FROM THE DEAN (FASCM)



**Prof. Dr. Ragavi V,
Dean, Faculty of Arts, Science, Commerce and Management (FASCM)**

It is my pleasure to note that Department of Chemistry & Centre for Material Chemistry, FASCM, Karpagam Academy of Higher Education are organizing the first International Conference on “Innovations in Material Chemistry for Sustainability (ICIMCS-2026)” from 18th to 20th February, 2026.

The venture is an initiative to setup a challenging research ambiance and to sculpt the standards of research. Keeping in mind the tremendous growth in the research field of Materials Chemistry and Sustainability, we strongly believe that the conference will not only lay a promising platform for the growth of research scholars but also to reinforce our place in the academia.

I wish the conference organizing team all the very best and grand success of the conference.

**Dean, FASCM
Karpagam Academy of Higher Education**

MESSAGE FROM DEAN (R&D and IR)



Prof. Dr. V. Parthasarathy
Dean, Research & Development and Industry Relations (R&D and IR)

The Karpagam Academy of Higher Education is honoured to host ANRF sponsored International Conference on “Innovations in Material Chemistry for Sustainability (ICIMCS-2026)” on February 18th to February 20th, 2026. It is truly inspiring to witness the overwhelming response from researchers and professionals across the globe, reflecting the significance of this conference in shaping the future of sustainable materials.

I extend my heartfelt gratitude to all the distinguished invited speakers for their invaluable presence and insightful contributions to this esteemed conference. I am confident that ICIMCS-2026 will serve as a dynamic platform for knowledge exchange, fostering meaningful discussions on cutting-edge advancements in Materials Chemistry and sustainability. With the participation of globally renowned experts delivering plenary lectures, keynote addresses and invited lectures, this conference promises to be a transformative experience for all attendees. The exchange of ideas and collaborations formed here will undoubtedly drive innovation and progress in this critical field.

My hearty wishes to the organizers of ICIMCS-2026 for their unwavering dedication and relentless efforts in making this conference a remarkable success.

Dean, R&D and IR
Karpagam Academy of Higher Education

MESSAGE FROM THE CONVENORS



**Dr. A. Thangamani,
Head, Department of Chemistry**



**Dr. K. Saravana Mani
Head, Centre for Material Chemistry**

We are glad to conduct the ANRF sponsored International Conference on “Innovations in Material Chemistry for Sustainability (ICIMCS-2026)” from 18th February to 20th February, 2026. We believe that this conference will be a great platform for innovative discussions and share ideas on materials chemistry and sustainability through plenary lectures, keynote lectures, invited lectures, oral and poster presentations.

The lectures and presentations will revolve around how we can leverage advanced materials to address current pressing issues such as environmental pollutions, generation of energy by sustainable technologies, and health concerns, while contributing to the realization of the Sustainable Development Goals (SDGs).

We are confident that the ideas exchanged at this conference will pave the way for a brighter, more sustainable future. We look forward to engage with all of you and work together to create innovative solutions that will drive global progress toward the Sustainable Development Goals.

Thank you for joining us in this crucial endeavor.

**Dr. A. Thangamani,
Head, Department of Chemistry
Karpagam Academy of Higher Education**

**Dr. K. Saravana Mani
Head, Centre for Material Chemistry
Karpagam Academy of Higher Education**

PROGRAMME SCHEDULE
First International Conference on “Innovations in Material Chemistry for Sustainability (ICIMCS-2026)”
Venue: *Umapathi Sivam Hall, Karpagam Academy of Higher Education*



Day – 1 (18.02.2026) Wednesday		
8:30 AM onwards	Registration	
9: 00 – 10:30 AM	INAUGURATION	
10:30 -11:00 AM	PHOTO-SESSION AND HIGH TEA	
Session Chairperson	Dr. K. Gopal, PSG College of Arts and Science, Coimbatore	
11:00 - 11:45 AM	PL-01: Prof. R. Murugavel Indian Institute of Technology Bombay, India	Topic: <i>Confluence of Metal Phosphate Molecules and Nanomaterials for Energy Transition: Selected Examples</i>
11.45 AM – 12.30 PM	IL-01: Prof. Biji Pullithadathil PSG Institute of Advanced Sciences	Topic: <i>Advanced Carbon Support Engineering for High-Performance and Durable PEMFC Electrocatalysts</i>
12:30- 13:30 PM	LUNCH BREAK	
Session Chairperson	Dr. K. Balaji, PSG Itech, Coimbatore	
13:30 -14:30 PM	POSTER SESSION-1: PP – 01 to PP – 40	
13.30-15.30 PM	*ORAL SESSION-1: OP – 2 to OP – 15 Session Chairperson: Dr. M. Karunakaran, Alagappa Government Arts College, Karaikudi.	
14:30 – 15:15 PM	KL-01: Prof. Ramesh Kasi Universiti Malaya, Malaysia	Topic: <i>Multifunctional Natural Rubber Hydrogel Electrolytes for Stretchable and Self-Healing All-in-One Supercapacitors</i>
15:15 – 16:00 PM	KL-02: Prof. Venkata Krishnan Indian Institute of Technology, Mandi	Topic: <i>Development of Sustainable Heterogeneous Catalysts for Energy and Environmental Applications</i>
16:00 – 16:15 PM	Contributed Invited Talk 1: Dr. S. Rajalakshmi (OP-1)	Topic: <i>From Sustainable Materials to Human Health: Rethinking Air Pollution Mitigation through Interdisciplinary Chemistry</i>
16:15 -16:30 PM	HIGH TEA	

PL – Plenary Lecture; IL – Invited Lecture; KL – Keynote Lecture; *Parallel session

PROGRAMME SCHEDULE
First International Conference on “Innovations in Material Chemistry for Sustainability (ICIMCS-2026)”
Venue: *Umapathi Sivam Hall, Karpagam Academy of Higher Education*

Day – 2 (19.02.2026) Thursday		
8:30 onwards	Registration	
Session Chairperson	Dr. Muthulakshmi Andal, PSGR Krishmmal College for Women, Coimbatore	
9:00 – 9:45 AM	PL-02: Prof. Vijayamohan K Pillai IISER Tirupati	Topic: <i>Impact of Two-Dimensional (2D) Materials as Quantum Dots for Energy Storage</i>
9:45 – 10:30 AM	KL-03: Prof. Kothandaraman Ramanujam Indian Institute of Technology, Madras	Topic: <i>Reinforcing a Lithium-ion Battery Cathode (NCA) with Mn Doping</i>
10:30 -11:00 AM	PHOTO-SESSION AND HIGH TEA	
Session Chairperson	Dr. Debabrata Barik, Professor, Dept. of Mechanical Engineering, KHAE	
11:00 - 11:45 AM	KL-04: Prof. Rajadurai Chandrasekar University of Hyderabad	Topic: <i>Molecular Crystals as New Materials for Photonic Circuits and Visible Light Communication</i>
11.45 AM – 12.30 PM	IL-02: Dr. Narendra Kurra Indian Institute of Technology, Hyderabad	Topic: <i>MXenes: Emerging Charge Storage Hosts for Multivalent Metal-Ion Storage</i>
12:30- 13:30 PM	LUNCH BREAK	
Session Chairperson	Dr. B. Janarthanan, Professor & Head, Dept. of Physics, KAHE	
13:30 -14:30 PM	POSTER SESSION – 2: PP – 41 to PP – 80	
13.30-15.30 PM	*ORAL SESSION-2: OP – 16 to OP – 30	
14:30 – 15:15 PM	KL-05: Prof. Sankarasekaran Shanmugaraju Indian Institute of Technology, Palakkad	Topic: <i>Emerging Functions of Tröger’s Base-Amino-1,8-Naphthalimides in Supramolecular Materials Design</i>
15:30 – 16.15 PM	TEA BREAK	
16:15-17:00 PM	KL-06: Dr. Nikhil Koratkar Rensselaer Polytechnic Institute, United States	Topic: <i>Battery Electrodes: Nano vs Micro-Structuring</i>

PL – Plenary Lecture; IL – Invited Lecture; KL – Keynote Lecture; *Parallel session

PROGRAMME SCHEDULE
First International Conference on “Innovations in Material Chemistry for Sustainability (ICIMCS-2026)”
Venue: Umaphathi Sivam Hall, Karpagam Academy of Higher Education

Day – 3 (20.02.2026) Friday		
8:30 onwards	Registration	
9:00 – 10:00 AM	PL-03: Prof. S. Sampath Indian Institute of Science, Bangalore	Topic: <i>Towards Sustainable Materials for Electrochemical Energy Conversion and Storage</i>
10:00 -10:30 AM	PHOTO-SESSION and HIGH TEA	
Session Chairperson	Dr. S. N. Karthick, Bharathiar University, Coimbatore	
10:30 – 11.15 AM	IL-03: Dr. Shanmugavel Chinnathambi Kyoto University, Japan	Topic: <i>Smart Fluorescent Nanomaterials for Biomedical Applications</i>
11:15 AM- 12:00 PM	KL-07: Prof. Azhagamuthu Muthukrishnan IISER Trivandrum	Topic: <i>Metal-free Electrocatalysts: Defects vs Heteroatom(s)</i>
12.00 – 13:30 PM	ORAL SESSION -3: OP – 31 to OP – 38	
12:30- 13:30 PM	LUNCH BREAK & POSTER SESSION -3: PP – 81 to PP – 119	
13:30-14:30 PM	VALEDICTORY	
14:30 -15:00 PM	PHOTO-SESSION and HIGH TEA	

PL – Plenary Lecture; IL – Invited Lecture; KL – Keynote Lecture;

TABLE OF CONTENT

LECTURES		
No.	Title	Page No.
Plenary Lectures		
PL-01	Confluence of Metal Phosphate Molecules and Nanomaterials for Energy Transition: Selected Examples. Ramaswamy Murugavel	1
PL-02	Impact of Two Dimensional (2D) Materials as Quantum Dots for Energy Storage. Vijayamohanan K Pillai	2
PL-03	Towards Sustainable Materials for Electrochemical Energy Conversion and Storage. S. Sampath	3
Invited Lectures		
IL-01	Advanced Carbon Support Engineering for High-Performance and Durable PEMFC Electrocatalysts Biji Pullithadathil	4
IL-02	MXenes: Emerging charge storage hosts for multivalent metal-ion storage. Narendra Kurra	5
IL-03	Smart Fluorescent Nanomaterials for Biomedical Applications Shanmugavel Chinnathambi	6
Keynote Lectures		
KL-01	Multifunctional Natural Rubber Hydrogel Electrolytes for Stretchable and Self-Healing All-in-One Supercapacitors. Ramesh Kasi	7
KL-02	Development of Sustainable Heterogeneous Catalysts for Energy and Environmental Applications. Venkata Krishnan	8
KL-03	Reinforcing a Lithium-ion Battery Cathode (NCA) with Mn Doping Kothandaraman Ramanujam	9
KL-04	Molecular Crystals as New Materials for Photonic Circuits and Visible Light Communication. Rajadurai Chandrasekar	10
KL-05	Emerging Functions of Tröger's Base-Amino-1,8-Naphthalimides in Supramolecular Materials Design. Shanmugaraju Sankarasekaran	11
KL-06	Battery Electrodes: Nano vs Micro-Structuring Nikhil A. Koratkar	12
KL-07	Metal-free Electrocatalysts: Defects vs Heteroatom(s) A. Muthukrishnan	13

ORAL PRESENTATIONS		
OP No.	Title	Page No.
OP-01	From Sustainable Materials to Human Health: Rethinking Air Pollution Mitigation through Interdisciplinary Chemistry, Subramaniyam Rajalakshmi*	14
OP-02	Dual-Function Modified g-C ₃ N ₅ Nanodots for Ultra-Sensitive Luminescent Detection and Complete Degradation of Ciprofloxacin. Raghul Ramachandran, Ajayan Vinu*, Bernaurdshaw Neppolian*	15
OP-03	Hesperetin:4-Aminopyridine Cocrystal (2HSRT:4AP)-A Strategy for Improving Solubility, J. Roshni, T. Karthick*	16
OP-04	Supramolecular Crystal Engineering Approach for Assembling 18-Crown-6 Ether (C ₁₂ H ₂₄ O ₆) 4-Aminopyridinium Perchlorate Complex (C ₅ N ₂ H ₃ ⁺ .ClO ₄ ⁻) for Nonlinear Optical Applications. S. Sai Suruthi, K.C. Lalithambika*	17
OP-05	Mononuclear Palladium(II) Hydrazone Complex: Synthesis, Characterization and In Vitro Cytotoxicity towards Human Cancer Cells. Balathandapani Narayanan, Ramasamy Uthayamalar, Datchinamoorthy Thirupathi, Ganesan Ayyannan, Gunasekaran Raja*	18
OP-06	Uniform Coating of NiO-Nanoparticles on Diamond Particles as Efficient and Stable Catalyst for Hydrogenation of Carbonyl Compounds. Datchinamoorthy Thirupathi, Ramasamy Uthayamalar, Balathandapani Narayanan, Ganesan Ayyannan, Gunasekaran Raja*	19
OP-07	Peripherally Fluorinated Tetraphenylethene: New Electron Extraction Interlayers for n-i-p Perovskite Solar Cells. Yamuna Ezhumalai, Ming-Chou Chen*	20
OP-08	An ESIPT-Active TREN-1,8-Naphthalimide Schiff Base Fluorescent Probe for Selective Zn(II) Sensing and Bioimaging. Ruhila Taj M, Mannanthara Kunhumon Noushija, Sankarasekaran Shanmugaraju*	21
OP-09	Tröger's Base Containing N-Rich Porous Metal-Organic Frameworks for Selective and Enhanced Adsorption of CO ₂ , Raju Saravanan, and Sankarasekaran Shanmugaraju*	22
OP-10	Gd-Doped NiWO ₄ Heterostructures with ZnO and ZnSe for Enhanced Charge Transport and Electrocatalysis. Sanjay N, Manikandan A and Rajendran TV*	23
OP-11	Synergistic Heterointerface Engineering of Ti ₃ C ₂ Tx/g-C ₃ N ₄ Bilayers for Robust Sn-Based Alloying-Type Negatodes for Sodium-ion Pouch Batteries. Lakshmanan Sathishkumar, Sambedan Jena, Duy Thanh Tran, Nam Hoon Kim*, Joong Hee Lee*	24
OP-12	Computational Multi-Target Drug Discovery Pipeline for Diabetic Foot Ulcer Targeting VEGFR2, MMP-2/9, NF-κB, and IL-1β. Xavier Prisil Naveentha, Govindasamy Rathika*	25

OP-13	An Artificial Intelligence-Powered Prediction and Optimization of Biogas Yield from Agro-Residues for Sustainable Energy. J. Saranya*, Y. Jeevan Nagendra Kumar, Y. Ram Lohit Pranay	26
OP-14	Negative Electrode for Next Generation Energy Storage Device. S.P Soumya Ranjan Nayak, S. Sharmila*	27
OP-15	Design and Thermal Performance of Imidazole-Functional Benzoxazine/Epoxy Hybrid Polymer Networks, Pavithra Panneerselvan, Devaraju Subramani, Alagar Muthukaruppan, Venkateswaran Ramalingam*	28
OP-16	A Naphthyl-Based Turn-on Fluorescent Chemosensor for Dual Detection of Ba ²⁺ Ions and Mancozeb. S. Kavanya, G. Narmatha, Elizabeth Antony, R. Nandhakumar*	29
OP-17	Design of a Uryl-Based Chemosensor for Dual Colorimetric and Fluorimetric Detection of Toxic Hg ²⁺ Ions and Amino Acids. S. Veeramani, S. kavanya, J. Prabhu, R. Nandhakumar*	30
OP-18	Mono Nano-Probe, Duo Signals: Dual Colorimetric and Fluorescent Detection of Dimethoate and Chlorpyrifos. Lokashree Dharmalingam, S. Veeramani, B. Vidhya, R. Nandhakumar*	31
OP-19	Temperature-Dependent Lattice Dynamics of Barium Zirconate Using First-Principles Quasi-Harmonic Phonon Calculations. Prabhakaran Manoharan, Raja Nadarajan*	32
OP-20	2D Amphiphilic Janus silica from natural clay as sustainable Pickering emulsifier. Pon Nivetha Ambiheswaran, Lalitha Pottail*	33
OP-21	Super Capacitors the Future for Energy Storage Lokeswari M, Sivashankari C*	34
OP-22	Interfacial Design of 1T-MoS ₂ /Co ₃ O ₄ Composite for Enhanced Electrocatalytic Oxygen Evolution Reaction. Angappan Jayanthi, Subramaniam Jayabal*	35
OP-23	Cascade Synthetic Strategy Toward Novel Triazoles: SAR Analysis and Molecular Modeling Insights. Prathiksha A, Jeyachandran M*	36
OP-24	Magnesium Salt-Doped Pectin/Guar Gum Electrolytes: A Bio-Based Approach to Energy Storage Materials. Nandhini Dhanavel*, Saratha Raman, Shilpa Rajendran, Thrisha Krishnasamy	37
OP-25	E-Waste as a Circular Resource: Sustainable Metal Recovery Technologies and Material-Centric Challenges for Circular Economy Applications. Annu Kumari, Dr. Sivasankari C*, Mahalakshmi R	38
OP-26	Fabrication of Novel Bi ₂ MoO ₆ /Nb ₂ CTx Schottky Heterojunction Photocatalyst Toward Efficient Antibiotic Degradation. Kandasamy Sasikumar, Ramar Rajamanikandan, Heongkyu Ju*	39
OP-27	An Ultrasensitive Chromone-Derived Fluorescent Chemosensor for Cu ²⁺ Detection Through LMCT: Real-World Applications and Computational Insights. P. Nivetha, A. Thangamani*	40

OP-28	Salt-Dependent Ionic Transport in Sodium Alginate Polymer Electrolytes: A Comparative Study of Sodium Bromide and Sodium Nitrite for Sodium-Ion Batteries. K. Thrisha*, R. Saratha	41
OP-29	Interfacial Charge Transfer and Oxygen-Vacancy Effects in Pd-Engineered ZnO during Ciprofloxacin Photodegradation. M. Tiffany, V. Pandiyan*	42
OP-30	Membrane-Assisted Light-Adaptive Sm–ZnO Photocatalyst for Antibiotic and Dye Abatement Coupled with Efficient Pathogen Suppression. T. Abisheik, V. Pandiyan*	43
OP-31	Antimicrobial Characteristics of Molecular Complexes of Zn(II) and Cd(II) Metal Ions. Lakshmi Krishnaa Suresh, Simi M, Santhy A, Kandasamy Gopal*	44
OP-32	Environmental Remediation of Heavy Metals from Effluents Through Metal Organic Frameworks. B. Nandini, P. Madhumitha, M. Amutha Selvi*	45
OP-33	Rational Design of MoWS ₂ /NiMoO ₄ Hybrid Electrodes with Enhanced Interfacial Coupling for Energy Storage Applications. T. Epsiba, A. Manikandan*	46
OP-34	Development of Value-Added Carbon Dots from Renewable Plant Waste at PSGCAS through Green Method for Real Time Bioimaging Applications, T. Kavitha, M. Keerthana	47
OP-35	Bio-Derived Trifunctional Sustainable Benzoxazines for Corrosion Protection and Multifunctional Surface Applications, Krishnakumar Arumugam, Balaji Krishnasamy*, Kailasam Saravana Mani	48
OP-36	Synthesizing a Luminescent Copper Metal-Organic Framework and Utilizing It for the Fluorescent Detection and Discrimination of Ethanol and Methanol. Thejaswini Rajesh, V. Madhu*	49
OP-37	Electrolyte-Driven Modulation of Redox Kinetics Governing Charge Storage in Copper Manganese-based Prussian Blue Analogues for Aqueous Potassium-Ion Batteries. Muthu Chandru Sundaram, Manik Clinton Franklin, Lekshmi Sunil, Imani Sospeter, Hemalatha Kuzhandaivel, Karthick Sivalingam Nallathambi*	50
OP-38	Dielectric and Conductivity Studies of <i>Pterocarpus marsupium</i> Gum Doped with NaClO ₄ . D. Catherine Denisha, S. Anna Venus, Manikandan Ayyar	51

POSTER PRESENTATIONS		
PP No.	Title	Page No
PP-01	Green-Synthesized B/N co-Doped Carbon Quantum Dots for Dual Fluorescence Sensing of Phenothiazine Drugs and Hg ²⁺ Ions S. Viji, K. Radhakrishnan*, A. Manikandan*, G. Ramachandran	52
PP-02	CeO ₂ Nanoparticles Decorated on CoAl-LDH Hexagonal Nanosheets as a High-Performance Hybrid Electrode for Supercapacitors K. Sareena, B. Kavitha*, A. Manikandan*	53
PP-03	New Insights into Continuous Flow Reactor Systems for the Effective Degradation of Persistent Pharmaceutical Pollutants Using Advanced Oxidation Processes Jeyaprakash Jenson Samraj, Bernaurdshaw Neppolian*	54
PP-04	Nitro Quinolone Fused Salicyl and Naphthyl Hydrazone Fluorescent Probes for the Detection of Fe ³⁺ and Pb ²⁺ Ions R. Mahalakshmi, R. Sentamil Selvi, N. Vandana, T. Suresh*	55
PP-05	Ligand-Engineered Homoleptic Co(III) Complexes Based on Salicylamine-Schiff Bases for Oxygen Evolution Electrocatalysis Murugesan Muthumeena, Janardhanan Aiswarya, Balasubramanian Murugesapandian*	56
PP-06	Quinoline-Dipeptide Conjugated Scaffolds as Effective Uric Acid Sensors M. Jayavani*, G. Selvi	57
PP-07	Applications of Click Chemistry in Modern Drug Discovery and Targeted Drug Delivery: A Review B. Saranya*	58
PP-08	The Effect of the Unsaturated Polyester Resin in Carbon Doped MgO as a Electrocatalyst in the Aluminium Air Battery. Aneesha S. A., Madhuradevi T., Dhanus Kumar Bharathamani, Ravi Subban*	59
PP-09	Analytical Investigation of Synthetic Polymer Exposure in Wildlife Using FTIR and Thermogravimetric Techniques N. Srinivasan, R. Nandhakumar, J. Prabhu*	60
PP-10	In-Vitro Studies of PVA-Chitosan Nanofibers Infused with Neem and Aloe vera for Advanced Antimicrobial Protection K. Abitha, B. Aishwarya, Nimisha, H. Jayalekshmi, K. S. Rajni*	61
PP-11	Tungsten-Cobalt Oxalate with Multiple Catalytic Sites as Efficient Electrocatalyst for Boosting Overall Water Splitting M. Padmavathy*	62
PP-12	Synergistic Integration of LaMnO ₃ @NiCo ₂ O ₄ Heterostructures with rGO for Efficient Hybrid Supercapacitors H. Gayathri, A. Pandurangan*	63
PP-13	Green Conversion of Carbon Dioxide to Formic Acid via Metal Complex Catalyzed Hydrogenation M. Usha Ramani*, J. Joseph	64

PP-14	Metal Carbamate Complexes as Cholinesterase Inhibitors: An ANN-Based Predictive Study K. Nagashri* ,V. Mariammal	65
PP-15	A Novel Schiff base - based Fluorescent Chemosensor for Al ³⁺ Ion Detection in Aqueous Solution R. Kavitha*	66
PP-16	Biogenic Bandgap Engineering of Cu Infused TiO ₂ : Comparison Of Structural Evolution of Leaf and Seed Fusion Routes *Deepthy P Nair, E.Sivasenthil*	67
PP-17	Synthesis, Characterisation and Pigment Studies of Cobalt-Doped Bismuth oxide (Bi ₂ O ₃) Nanoparticles P. Subhashree, B. Pavithra, R. Suresh, A. Vijayaraj*	68
PP-18	Structural, Spectroscopic and Optical Properties of LTF Single Crystals: Comparative Approach Nandhini Ramu, Sivasenthil Elangeeran*	69
PP-19	Synthesis and In-Silico Biological Evaluation of 3-Substituted 2-Selenoquinoline Derivatives to Cyclooxygenase Enzymes (COX-I and II) R. Revathi*, K. Saravanamani	70
PP-20	Valorization of Bio-Litter into Cellulose Adsorbents for Lead (II) Water Treatment N. Shyamala devi*, C. Swathi Sri	71
PP-21	Investigation of Strontium Ferrite Nanoparticles using Hydrothermal Approach for Photocatalytic Degradation of Methylene Blue Dye R. Mamani*	72
PP-22	Ultrasml N/S-doped Nb ₂ C MXene Quantum Dots as a Fluorescent “Turn-off” Platform for Sensitive Chloramphenicol Sensing in Food Samples Ramar Rajamanikandan, Kandasamy Sasikumar, Heongkyu Ju*	73
PP-23	Synthesis, Structural Characterization and Biological Evaluation of New Nickel (II) Complexes Containing Coumarin Based Schiff Bases R. Veerasamy, G. Kalaiarasi*	74
PP-24	Pigment Characteristics of Nickel Ferrite Powders O.A. Sridevi, M. Priyadharshini, R. Suresh*	75
PP-25	Photo-Fenton-like Catalytic Property of Fe ₂ O ₃ /Bi ₂ O ₃ Composite P. Kalpana, M. Priyadharshini, R. Suresh*, N. Jayaprakash	76
PP-26	Effect of ZnSrFe ₂ O ₄ Content on Magnetic and Dielectric Properties of Poly(o-phenylenediamine)/ZnSrFe ₂ O ₄ Nanocomposites M. Rajendra kumar, M. Mohanraj*	77
PP-27	Preparation, Electrical and Magnetic Properties of Poly(o-phenylenediamine)/CrSrFe ₂ O ₄ Nanocomposites A.Santhavignesh, M. Mohanraj*	78
PP-28	Synthesis, Structural, Magnetic and Electrical Characterization of Poly (o-phenylenediamine)/BaSrFe ₂ O ₄ Nanocomposites B. Gowthaman, R. Rajkumar*	79
PP-29	Investigation of Magnetic and Dielectric Properties of Poly (o-phenylenediamine)/CuSrFe ₂ O ₄ Nanocomposites P. Navin, R. Rajkumar*	80

PP-30	Harnessing Cd-doped ZnO Nanoparticles for Solar and UV-C induced Azo Dyes Degradation and Broad-Spectrum Antibacterial Activity T. Dhivya, V. Pandiyan*	81
PP-31	Zr-modified ZnO Nanoparticles: Optimized Photocatalytic Degradation and Antibacterial Efficiency for Pollution Control V. Dhivyadharshini, V. Pandiyan*	82
PP-32	Study of Magnetic and Electrical Properties of Poly (o-phenylenediamine/NiSrFe ₂ O ₄) Nano Composites P. Pavithra, M. Mohanraj*	83
PP-33	Investigation of Magnetic, Dielectric and Thermal Properties of Poly (o-phenylenediamine)/SrCuFe ₂ O ₄ Nanocomposites N. Madhunisha, M. Mohanraj*	84
PP-34	Poly (o-Phenylenediamine)/CuCrFe ₂ O ₄ Nanocomposites: Synthesis, Structural Characterization, Thermal, Magnetic and Electrical Properties M. Pethanraj, R. Ravikumar*	85
PP-35	Synthesis, Structural, Electrical and Magnetic Properties of Poly (o-Phenylenediamine)/ BaCrFe ₂ O ₄ Nanocomposites V. Vignesh, R. Ravikumar*	86
PP-36	Oxygen-Rich Biomass-Derived Carbon Dots for Sensitive Fluorescent Detection of Ciprofloxacin in Water R. Mahalakshmi, K. Radhakrishnan*	87
PP-37	Nitrogen-Phosphorus Co-Doped Amino-Rich Biomass-Derived Carbon Dots as Green Fluorescent Probes for Malathion Detection G. Santhi, V. Prakash, K. Radhakrishnan*	88
PP-38	A Review on Green Synthesis of ZnO Nanoparticles - An Ecofriendly Approach K. Swathi*, R. Ravikumar	89
PP-39	Synthesis, Structural Characterization, Thermal, Magnetic and Electrical Properties of CuCrFe ₂ O ₄ Nanocomposites M. Mohanraj*, R. Ravikumar	90
PP-40	Electrical and Magnetic Properties of Poly (O-Phenylenediamine)/CrCoFe ₂ O ₄ Nanocomposites K. S. Selvavelan*, M. R. Ezhilarasi	91
PP-41	Green Synthesis of Lead-Tin Metal Oxide Nanoparticles using Euphorbia Hirta Plant Extract P. Sre Hariny, K. Rithika, M. R. Ezhilarasi*	92
PP-42	Sulfur-Doped Quantum Dots Integrated Fluorescent Sensor for Ultra-Sensitive Detection of Malathion Pesticide in Food Samples P.T. Balaji, K. Kulathuraan*	93
PP-43	Synthesis, Characterization and Environmental Application of CoSrFe ₂ O ₄ /Poly(o-phenylenediamine) Nanocomposites S. Avinash, M. Mohanraj*	94
PP-44	Boron-Doped Carbon Dots as Visible Light Responsive Nanocatalysts for Efficient Photocatalytic Degradation of Ciprofloxacin in Aqueous Systems. J. Sagaya agnes nisha¹, K. Kulathuraan	95

PP-45	Synthesis of Anticancer Agents: Molecular Docking and ADME Studies of New Hydopyrimidine Linked Amide-Pyridine Derivatives Rajendran Aarthi, Chin-King Looi, Chun-Wai Mai, Chennan Ramalingan	96
PP-46	Chitosan Integrated CuAl LDH: A Sunlight Competent and Recoverable Photocatalyst for Nitrofurantoin Degradation Kannan Ajitha, Vadivel Saravanan, Chenan Ramalingan*	97
PP-47	Plant-Based Synthesis of Lead-Tin oxide nanoparticles using Euphorbia Hirta plant extract. Rithika. K, Sre Hariny P and Ezhilarasi M.R*.	98
PP-48	Green Synthesis of Silver-Ion-Embedded Chitosan–PVA Nanocomposite Films Using Leucas aspera Leaf Extract for Antimicrobial Food Packaging Applications. R. Janani, B. Supriya, P. Kavitha, R. Menaka	99
PP-49	Development of Eco-Friendly Chitosan–PVA Based Nanocomposite Film Incorporated with Silver Ions for Antimicrobial Food Packaging Applications. B. Supriya, R. Janani, P. Kavitha, R. Menaka	100
PP-50	Fluorescent Detection of Carbamate Pesticides Using Biomass-Derived Nitrogen–Sulfur Co-Doped Carbon Dot@ZnO Nanocomposites V. Prakash, K. Radhakrishnan*, G. Santhi	101
PP-51	Design and Fabrication of CuMoO ₄ /NiO as an Advanced Electrode for Hybrid Supercapacitors S. Sakthivel, Manikandan Ayyar*	102
PP-52	Cobalt Vanadate Anchored on Reduced Graphene Oxide: A high-Performance Electrode Material for Supercapacitors B. Kabilan, A. Manikandan*	103
PP-53	Rapid Portable Detection of Chemical Warfare Agent Mimic Diethyl Chlorophosphate (DCP) using a Rhodamine-Quinoline Conjugated Probe with Fluorescent “Turn-on” and Chromogenic Responses, and Cancer Cell Imaging K. Kaviya, K. Saravana Mani*	104
PP-54	Conducting Bimetallic MOF Derived Nitride: A Unique Pathway for the Transformation of Amorphous to Metallic MOF Ashamary Francis, Manoj Devaraj*	105
PP-55	Thermal Synthesis of Fe ₂ O ₃ /ZnFe ₂ O ₄ Composite Photocatalyst M. Priyadharshini, R. Suresh*,	106
PP-56	Polymer Electrolyte Membrane for Fuel cell Applications N. Nithya, B. Kavitha, A. Manikandan	107
PP-57	Design of Quinoline-Amide Conjugates Targeting HPV-mediated Proteins to Suppress Cervical Cancer R. Susheela, K. Saravana Mani	108
PP-58	Multicomponent Synthesis and Structure of Novel Spiroindanedione-pyrroloisoquinolines by 1,3-dipolar Cycloaddition of Azomethine Ylide S. Krithika, A. Thangamani*	109

PP-59	Multifunctional MWCNT Enriched Nickel Cobalt Sulfides Composites for High-Performance Supercapacitors and Dye-Sensitized Solar Cells V. Gayathri, R. Suresh, C. Rajamohan*	110
PP-60	Cellulose Acetate/SrO Composite Biopolymer Membranes: Structural, Functional and Thermal Analysis R. Gayathri, S. Sharvasri, Aparna Unnikrishnan, J. Balavijayalakshmi*	111
PP-61	Bimetallic MOF Coated Screen Printed as Disposable Electrode for Electrochemical Detection of Paracetamol Muruganantham Purushothaman, Devraj Manoj*	112
PP-62	Limit to DNA Reactive Substances in Drug Substances and in Drug Products Lenin Kumar K, Dhanus Kumar Bharathamani, Ravi Subban*	113
PP-63	One-pot Multicomponent Synthesis of Bioactive Dispiro-indenoquinoxaline Pyrrolidine Derivatives Bismi Rani I V, A. Thangamani*	114
PP-64	Process Development of (2S,3R)-1-(Dimethylamino)-3-(3-Methoxy phenyl)-2-Methyl Pentan-3-ol V. Vijayalakshmi, Ravi Subban*, Venkata Reddy, A. Thangamani	115
PP-65	Dual-mode Schiff Base Chemosensor for Selective Detection of Cu ²⁺ and Zn ²⁺ in DMSO: Mechanism and Practical Applications S. Kamalpathi, P. Nivetha, A. Thangamani*	116
PP-66	Photocatalytic Degradation of Oxytetracycline Using Co-Cu Co-doped Al ₂ O ₃ @Fe ₂ O ₃ Nanocomposites V. Suguna , K. Sundaram*	117
PP-67	A Dual-channel Chemosensor Based on Carbazole Based Schiff Base for Fluorescence Detection and Colorimetric Recognition of Glutamic Acid B. Priyadharshini, P. Nivetha, A. Thangamani*	118
PP-68	Dielectric and Morphological Analysis of Poly (m-phenylenediamine)/CoMnFe ₂ O ₄ Nanocomposites V. Mahasakthi, N. Kannapiran*	119
PP-69	Investigation on Cu-doped BiLaO ₃ Nanoparticle as a Potential Effluent Treatment of Photocatalysis Dye Degradation Ananya Sasikumar, Manikandan Ayyar*	120
PP-70	A Highly Selective Ratiometric and Colorimetric Detection of Ni ²⁺ and Co ²⁺ ions using Schiff Base Ligand B. Yogarajan, P. Nivetha, A. Thangamani*	121
PP-71	Synthesis of Polymer/ZnNiFe ₂ O ₄ Nanocomposites for Dielectric Applications R. Pravin Bathma Priya, R. Kumar*	122
PP-72	Luminescence sensing, DFT, Extraction and Monitoring of Cr ³⁺ and Al ³⁺ Via the Application of First Derivative Fluorescence Spectroscopy T. Mugilarasu, P. Nivetha, A. Thangamani*	123
PP-73	Fe ₂ O ₃ /BaSO ₄ Nanocomposite: Preparation, Characterization and Pigment Property Abdul Saleem M, R. Suresh*	124

PP-74	Thermal and Morphology Analysis of Poly(m-phenylenediamine) /NiMnFe ₂ O ₄ Nanocomposite B. Muruges, N. Kannapiran*	125
PP-75	Photocatalytic Degradation of Antibiotics using Zn–Fe Doped CuO Nanoparticles M A. Junaid, K. Sundaram*	126
PP-76	The Effect of Carbon Doped Magnesium Oxide with Thorium Electrocatalyst in the Aluminium Air Battery S. Akilan, T. Pavithra, Dhanus Kumar Bharathamani, Ravi Subban*	127
PP-77	The Effect of the Coconut Coir Carbon doped Zirconium Oxychloride Octahydrate with Epoxy Resin as Cathode Material in Aluminium Air Battery S. Karthick, Dhivya Madheswaran, Dhanus Kumar Bharathamani, Ravi Subban*	128
PP-78	Photocatalytic Properties of Fe ₂ O ₃ /g-C ₃ N ₄ Composite A.Dickson Arokiya Nishanth, R. Suresh*	129
PP-79	Evaluation of NIR Reflective Property of BiVO ₄ /BaSO ₄ Composites Rhushikesh Rajendran Jadhav, R. Suresh*	130
PP-80	Benzothiazole-Lepidine Based Fluorescent Probe for the Selective Detection of Cyanide in Solution U. Gokul, K Kaviya, K. Saravana mani *	131
PP-81	Recent Trends in Various Carbon Film/Materials and Cell Design for Aluminium Ion Battery D. Sam Wilfred, Ashik Devaraj, Dhanus Kumar Bharathamani, Subban Ravi*	132
PP-82	Amine Functionalization of Biochar for Tailoring Surface Charge and Enhancing Zero-point Charge (pHzpc) Shobanapriya Murugan, Koyeli Das, Chien-Yen Chen*	133
PP-83	Benzothiazole-based Fluorescent Receptor for the Selective Detection of Phosgene in Solution Dharani Tharan M, K Kaviya, K. Saravana Mani *	134
PP-84	Synthesis and Characterization of Poly(m-phenylenediamine) /ZnMnFe ₂ O ₄ Nanocomposites M. Arjun, N. Kannapiran*	135
PP-85	A Triphenylamine Based Probe for the Ratiometric Detection of Phosgene in Solution A. Deva Augustin, K. Kviya, K. Saravana Mani*	136
PP-86	Chemical Composition of the Essential Oil from Anisomeles Malabarica V. Sudha, Ravi Subban*	137
PP-87	Coumarin based Fluorescent Receptor for the Selective Detection of Environmental Hazardous Analytes S. Narayanan, K. Kaviya, K. Saravana Mani*	138
PP-88	Synthesis of Mn ₃ O ₄ @ZnO Nanocomposites Decorated Poly(m-Phenylenediamine) for Photocatalytic Dye Degradation Application S. Sakthivel, N. Kannapiran*	139

PP-89	Synthesis and Characterization of La-doped MgCo ₂ O ₄ Nanostructures for Supercapacitor Applications S. Yasodharan, T. Kavinkumar *, A. Manikandan1*	140
PP-90	Enhanced Visible-Light Photocatalytic Removal of Antibiotics Using Ag-Doped Rare Earth Cobaltate Nanostructures V. Vidhyasri, A. Manikandan*	141
PP-91	Degradation of Antibiotic using Cu-Al Co-doped MnO ₂ Nanocomposite A. S. Logesh, K. Sundaram*	142
PP-92	Sulfur–Phosphorus Co-Doped Carbon Dots for Turn-Off Fluorescence Detection of Chloramphenicol S. Bhuvanesh, K. Radhakrishnan*	143
PP-93	Synthesis and Characterizations of V ₂ O ₅ /FeOOH Composite Photocatalyst. S. Karthikaikannan, R. Suresh*	144
PP-94	Metal-Free Fluorescent Recognition of Glyphosate Using Biomass-Derived Nitrogen-Doped Carbon Dots. P. Dharani, K. Radhakrishnan*	145
PP-95	Synthesis and Characterization of Ni ₃ V ₂ O ₈ /Co-Cu LDH Nanocomposite for Supercapacitor Applications V. Rajadurai, A. Manikandan *	146
PP-96	Green-Synthesized Oxygen-Rich Carbon Dots for Enzyme-Free Fluorescence Detection of Organophosphate Pesticides through Hydrolysis-Induced Response K. Lithishkumar, K. Radhakrishnan*	147
PP-97	Development of Biodegradable Film for Advanced Wound Dressing and Wound Healing Applications R. Vishvapriya, Mouli Konar*	148
PP-98	Crystallographic Studies of Metal Complex using Heterocyclic and Organic Acids M. Mervin Joshua, Mohana*	149
PP-99	Structural and Electrochemical Insights into Ce ₂ (WO ₄) ₃ /g-C ₃ N ₄ Nanocomposites for Enhanced Supercapacitor Performance R. Mahalakshmi, D. Infant Jency, S. Esakki Muthu*, A. Manikandan	150
PP-100	Synthesis of Electrical and Morphological Analysis of Poly (m-Phenylenediamine)/CuMnFe ₂ O ₄ K. S. Jayashooreyaa, N. Kannapiran*	151
PP-101	Synergistic Effect of Co ₃ O ₄ Loaded g-C ₃ N ₄ /Bi ₂ MoO ₆ Ternary Heterojunction S-Scheme Photocatalytic Degradation of Malachite Green P. S. Moniga, A. Manikandan*	152
PP-102	Synthesis of Ivacaftor and Its Key Starting Material Using a Flow Process B. Jeeva, P. Senthil Kumar*	153
PP-103	Hierarchical Heterostructure of NiMoO ₄ as an Efficient Electrocatalyst for Water Splitting Kannushamy R, T. Kavinkumar*, A. Manikandan*	154

PP-104	Core-shell Structured Tungsten Disulfide/Zeolitic Imidazolate Framework-67 Nanocomposites as Cathode Material for Supercapacitor Application K. Sathish Kumar, V. Siva*	155
PP-105	Fast Modification of Porous Nickel Foam Substrate as Anode Material for Anion Exchange Membrane Water Electrolysis V. Abinaya, Pandiyarajan Anand*, Ching Wei Tung	156
PP-106	Degradation of Antibiotic using Ag-Mn co-doped NiO Nanocomposite R. Matheswaran, K. Sundaram*	157
PP-107	High-Energy Solid-State Synthesis of Sodium Manganese Oxide Nanobelts with Enhanced Electrochemical Performance M. Dineshkumar, A. Shameem*, V. Siva, A. Murugan	158
PP-108	Ultrasonic waves triggered CeO ₂ -hBN-g-C ₃ N ₄ heterojunction nanocomposites as a multifunctional electrode material for asymmetric supercapacitor and photocatalytic applications Z. Mohamed Riyas* Esakkimuthu Shanmugasundaram, A. Manikandan	159
PP-109	Green Synthesis of NiO and CuO Nanoparticles Using Vitis vinifera Extract for Photocatalytic Activity K. Priyadharshini, R. Kumar*	160
PP-110	Plant-Mediated Synthesis of ZnO, CuO and NiO Nanoparticles Using Cinnamon Extract and Investigation of Their Photocatalytic Efficiency G. Gayathri, R. Kumar*	161
PP-111	Green Synthesis of N/B Co-Doped Carbon Dots as π - π Stacking-Responsive Fluorescent Probes for Sensitive Detection of Carbendazim G. Aswin, K. Radhakrishnan*	162
PP-112	Bismuth Oxyhalides as Active Photocatalyst for Degradation of Methylene Blue under UV Light Irradiations R.G. Pradhoshram, Muruganantham Purushothaman, Devraj Manoj*	163
PP-113	Non-stabilized Azomethine Ylides in the Claisen Condensation: Synthesis of 5-Isatinylidenerhodanine Derivatives K. Muralidharan, A. Thangamani*	164
PP-114	Advanced Cathode Materials for Aluminum-Air Batteries: Metal Oxide/Activated Carbon Composites – A Comprehensive Review. R. Sangeetha and E. Sivasenthil	165
PP-115	Preparation and Characterization of a Composite made up of ZnO and Carbon obtained from Banana Peel as an Electrocatalyst for Aluminum-Air Battery. Dhanus Kumar Bharathamani, Naveenprakash R, Sangeetha R, Shandhiya Murugan, Ravi Subban, E. Sivasenthil*	166
PP-116	Synthesis, Structural Elucidation, Intermolecular and Non-Covalent Interaction Analysis, and Molecular Docking Studies of 3-Chloro-3-methyl-2,6-bis(4-methoxyphenyl)piperidin-4-one Picrate (CMMYPP) Arulraj Ramalingam*, Sivakumar Sambandam	167
PP-117	Transition Metal-Tuned MoS ₂ Nanostructures: Tailoring Structural Integrity and Emerging Optical Prospects. D. Infant Jency, S. Esakki Muthu*	168

PP-118	Engineering NiO incorporated MgMoV ₂ O ₆ Cathode material for Efficient Energy Storage Systems. D. Sher Meena, S. Anna Venus*, Manikandan Ayyar	169
PP-119	Fabrication, Characterization and Electrochemical evaluation of Pt-based Cathode Catalysts for Enhanced ORR in PEM Fuel cells. B. Delphine, S. Anna Venus, Manikandan Ayyar	170

PLENARY LECTURES [PL]
INVITED LECTURES [IL]
KEYNOTE LECTURES [KL]

| PL-01 |

Confluence of Metal Phosphate Molecules and Nanomaterials for Energy Transition: Selected Examples

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Abstract

Reaction of phosphoric acid mono- and diesters with a divalent transition metal ion can produce molecular clusters, 1-D polymers, 2-D grids, or 3-D frameworks. Particularly interesting among this series of structural types are the 1-D polymers that are built from thermally labile di-tert-butyl phosphate. These polymers with an inorganic backbone and organic sidechains readily and cleanly decompose at temperatures close to 200 °C. The nanomaterials produced from such precursors have been studied extensively as both electro- and photocatalysts in OER, HER, and overall water splitting reactions. The monoaryl phosphate, on the other hand, combines with Co^{2+} or Zn^{2+} in a donor solvent (L) leading to the isolation of tetranuclear metal phosphates $[(\text{R})\text{PO}_3\text{M}(\text{L})]_4$ (R = alkyl/aryl or alkoxy/aryloxy), whose inorganic core resembles the zeolitic D4R secondary building units (SBUs). In recent times, we have unravelled that it is possible to isolate even larger SBUs through small variations in the reaction conditions. Rationalization of building principles along with the use of this class of compounds for energy applications will be highlighted in this lecture.

For further representative publications, see: Murugavel & co-workers, *ACS Catalysis* **2023**, *13*, 8535; *Inorg. Chem.* **2022**, *61*, 6807 & **2020**, *59*, 13233; *J. Am. Chem. Soc.* **2017**, *139*, 39; *Chem. Commun.* **2019**, *55*, 7994; *Angew Chem., Int. Ed.* **2019**, 16844; *Small*, **2020**, 1903334; *Chem. Mater.* **2024**, *36*, 6475; *ACS Mater. Lett.* **2024**, *6*, 2126; *Chem. Asian J.* **2025**, e202401177; *Dalton Trans.* **2026**, *55*, 1306; *J. Mater. Chem. A.* **2026**, *14*, 1136; *Carbon*, **2026**, *249*, 121260.

| PL-02 |

Impact of Two Dimensional (2D) Materials as quantum Dots for Energy Storage

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Abstract

I have been working in the area of Materials Electrochemistry for about three decades starting my professional journey from NCL IISER – Tirupati via CSIR-CECRI. Preparation of different types of materials (monolayers to monolayer protected nanoclusters, nanowires and eventually polymer-nanocomposites) blending the synthetic skills of a Chemist with atomic molecular level characterization tools of condensed matter physicist was important but all most of all applications I explored were about electrocatalysis or electrochemical energy storage. My group dabbled up on diverse type of materials including zero-dimensional (quantum dots), one-dimensional (Carbon nanotubes), and two-dimensional (phosphorine) systems and their composites tailored for energy storage applications emphasising on their size/shape dependent properties. For example, most of the two-dimensional materials have a finite van der Waals gap (v-gap) in between the layers which provides a clear separation between the in-plane and through plane electronic interactions. Although the carrier transport and associated unique features are studied in accurately prepared and precisely characterized monolayers, many applications use multilayers which are conveniently prepared using inexpensive and scalable chemical methods. For example, among various two-dimensional (2D) materials, graphene possesses similar interlayer spacing of multiwalled carbon nanotubes (0.32–0.35 nm) which could be modulated by several strategies such as the intercalation of cations and anions, the nature of the solvent, and surface functionalization. The resultant graphene nanoribbons (~40 nm diameter) formed by the ionic liquid-assisted transformation of multiwalled carbon nanotubes of an average diameter (~21 nm) along with graphene quantum dots having an emission wavelength of 445 nm are more useful for some of the specific applications. The tunability of this spacing depends on the nature of the ionic liquid, the size of the incoming ions, the applied potential, and the time. In this lecture several examples electrochemically prepared 2D materials, their heteroatom doping and surface modification possibility will be discussed using both elemental and compound 2D quantum dots like Graphene, Phosphorene, carbon nitride, Molybdenum Sulphide, Bismuthene and clay based 2D composites will be demonstrated for specific applications like electrocatalysis and battery storage.

| PL-03 |

Towards Sustainable Materials for Electrochemical Energy Conversion and Storage

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Abstract

Our group has been interested in understanding various electrochemical interfaces relevant to energy conversion and storage, particularly using sustainable electrodes and electrolytes. This encompasses modified surfaces and electrodes involving materials as well as molecular assemblies. Our present interests include in situ electrochemistry at water-air interface under surface pressure, polymers and layered materials as electrodes to drive redox reactions relevant to rechargeable batteries, understanding solvent structure at an electrode-electrolyte interface, orientation dependent electrocatalysis etc. Organic and inorganic materials based on nitrides /carbides / layered chalcogenides and polymers are of current interest with respect to energy conversion and storage. The present lecture will discuss certain developments of the interfacial studies involving molecular systems and certain materials.

| IL-01 |

Advanced Carbon Support Engineering for High-Performance and Durable PEMFC Electrocatalysts

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Abstract

Polymer Electrolyte Membrane Fuel Cell (PEMFCs) have emerged as a promising clean energy conversion technology for automotive, portable, and stationary power applications due to their high efficiency, low operating temperature, and zero tailpipe emissions. Despite these advantages, large-scale commercialization remains constrained by the high cost and insufficient long-term durability of Pt-based electrocatalysts. A major limitation originates from the instability of conventional carbon supports under the harsh electrochemical conditions encountered during fuel cell operation, particularly at high potentials and during transient events. Carbon corrosion and associated structural degradation accelerate Pt nanoparticle agglomeration, dissolution, and detachment, ultimately leading to performance loss. This presentation highlights the rational design and engineering of advanced carbon-based catalyst supports as a viable strategy to simultaneously enhance catalytic activity and durability in next-generation PEMFC systems. Durability challenges under realistic operating conditions, including start–stop cycling and dynamic load fluctuations, are critically examined. The role of engineered carbon architectures in mitigating degradation pathways, such as carbon corrosion and platinum dissolution, is systematically discussed. Special emphasis is placed on tailoring surface chemistry, controlled mesoporosity, and heteroatom incorporation to regulate metal–support interactions, optimize Pt nanoparticle dispersion, and improve resistance to electrochemical oxidation. These design principles provide a framework for developing robust catalyst supports capable of sustaining high performance under practical fuel cell operating conditions.

| IL-02 |

MXenes: Emerging charge storage hosts for multivalent metal-ion storage

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Abstract

The emerging demand for affordable, clean, and sustainable electrochemical energy storage systems has fueled renewed interest in post Li-ion chemistries, relying on earth abundant materials and minerals. Specifically, multivalent metal ions (Zn^{2+} , Mg^{2+} , Ca^{2+} and Al^{3+}) can transfer two or more electrons per formula unit and exhibit superior volumetric capacities compared to monovalent metal-ions. However, their practical realization is hindered by sluggish ion diffusion kinetics, strong electrostatic interactions, and instability of the host materials during reversible (de)insertion. In the quest for suitable electrode materials, two-dimensional (2D) transition metal carbides, nitrides, and carbonitrides, known as MXenes, have emerged as promising charge storage hosts for multivalent ions. MXenes possess a unique combination of metallic conductivity, hydrophilicity, transition metal oxide/hydroxide redox chemistry and tunable interlayer spacing, which collectively enable fast and reversible multivalent ion storage. For instance, $\text{Ti}_3\text{C}_2\text{T}_x$ MXene exhibited proton-induced pseudocapacitive behavior in acidic electrolytes and intercalation-induced capacitive type charge storage behavior in neutral aqueous electrolytes, thus limiting charge storage capacities below 20 mAh g^{-1} . To overcome these intrinsic limitations, assemblies of $\text{Ti}_3\text{C}_2\text{T}_x$ with redox active organic molecules in forming organic-inorganic hybrid electrodes through electrostatic and hydrogen-bonding interactions were developed. These hybrid architectures enable enhanced pseudocapacitive charge storage in aqueous divalent metal-ion electrolytes. Pseudocapacitive charge storage behavior in vanadium carbide (V_2CT_x) MXene has been investigated through (electro)chemical surface modifications and electrolyte engineering using water-in-salt and salt-in-solvent electrolytes.

References

1. S. Yadav and N. Kurra, *Small*, 2025, 21, 2412429
2. S. Yadav and N. Kurra, *Batteries & Supercaps*, 2025, 10.1002/batt.202500305
3. S. Yadav and N. Kurra, *Energy Storage Materials*, 2024, 65, 103094.
4. S. Yadav and N. Kurra, *Journal of Materials Chemistry A*, 2024, 12, 32182.
5. S. Bhoi, S. H. Goudar, K. V. Rao, N. Kurra, *Cell Reports Phys. Sci.*, 2024, 5, 102229.
6. S. H. Goudar, S. Bhoi, K. V. Rao, N. Kurra, *Small*, 2024, 20, 2309905

| IL-03 |

Smart Fluorescent Nanomaterials for Biomedical Applications

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Abstract

Quantum dots (QDs) are nanoscale materials known for their exceptional optical and electronic properties, including tunable fluorescence, high quantum yields, and strong resistance to photobleaching. These features make them ideal candidates for multiplexed imaging and targeted drug delivery detection. Among various types, silicon and carbon-based quantum dots have emerged as especially promising for biological applications due to their high biocompatibility and safety profiles. Silicon quantum dots benefit from the material's widespread use in electronics and its natural compatibility with biological systems. Meanwhile, carbon-based quantum dots offer advantages such as excellent water solubility, low toxicity, environmental friendliness, and cost-effective synthesis, all while exhibiting desirable optical characteristics. In this presentation, both silicon and carbon quantum dots were employed for bioimaging in cells and medaka fish, as well as for tracking DNA-based drug delivery (Figure.1). The results demonstrate the potential of these quantum dots as effective and versatile fluorescent probes for a range of biomedical applications.

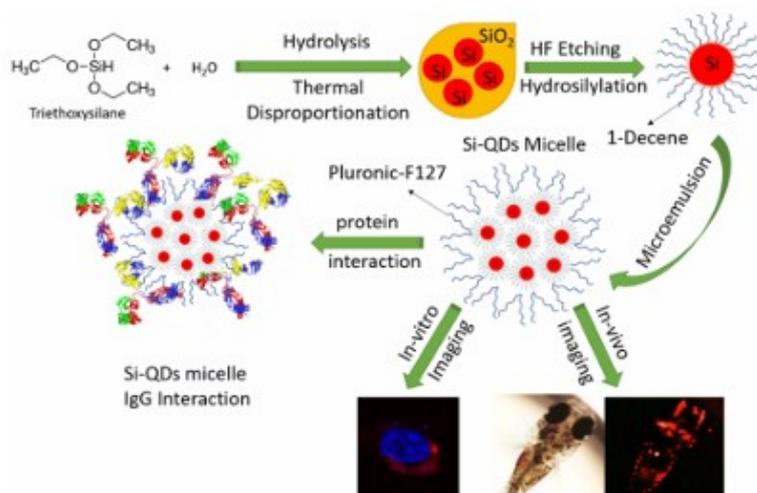


Figure 1. The schematic diagram illustrates the process of producing silicon quantum dots from the triethoxysilane precursor, which involves hydrosilylation with 1-decene and functionalization with Pluronic-F127. The resulting SiQD-De/F127 micelle is used as a safe and biocompatible staining agent in both in vitro and in vivo models. Additionally, a two-dimensional image demonstrates the interaction of IgG with the surface of the SiQD-De/F127 micelle.

| KL-01 |

Multifunctional Natural Rubber Hydrogel Electrolytes for Stretchable and Self-Healing All-in-One Supercapacitors

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Abstract

The increasing global energy demand and the intermittency of renewable energy sources require efficient energy storage technologies. Supercapacitors (SCs) offer high power density but are limited by low energy density, motivating the development of advanced multifunctional materials. This work presents the fabrication of high-performance all-in-one hydrogel supercapacitors based on natural rubber hydrogel electrolytes integrated with conducting polymers and metal oxide nanoparticles. Hydrogel electrolytes were synthesized via a free-radical mechanism using sodium montmorillonite (Na-MMT), glutaraldehyde (GA), and N,N'-methylene-bis-acrylamide (MBA) as cross-linkers, among which GA-based hydrogels exhibited superior ionic conductivity, mechanical properties, and swelling behavior. The optimized GA hydrogel was further treated in 1 M sodium sulfate (Na₂SO₄) for 24, 48, and 72 h to enhance charge carrier density, yielding GA24, GA48, and GA72 samples. Structural, chemical, and morphological characteristics were examined using XRD, FTIR, FESEM, and EDX, while ionic conductivity was evaluated by electrochemical impedance spectroscopy (EIS). GA48 demonstrated excellent stretchability, self-healing behavior, and the highest ionic conductivity of $1.94 \times 10^{-2} \text{ S cm}^{-1}$ at room temperature, making it the most suitable electrolyte for device integration. All-in-one hydrogel supercapacitors were subsequently fabricated via in situ polymerization of polyaniline (PANI) incorporated with titanium dioxide (TiO₂) and zirconium dioxide (ZrO₂) nanoparticles as electrode materials. Devices with varying metal oxide contents were evaluated using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and EIS, with PT35 (35 mg TiO₂) and PZ35 (35 mg ZrO₂) identified as the best-performing systems. The novelty of this work lies in the synergistic integration of a self-healing, salt-optimized natural rubber hydrogel electrolyte with PANI-metal oxide nanocomposites to realize a fully integrated, mechanically robust all-in-one supercapacitor architecture.

Keywords: All-in-one hydrogel, supercapacitor, Titanium dioxide, Zirconium Oxide, Hydrogel electrolytes, Natural rubber

| KL-02 |

Development of Sustainable Heterogeneous Catalysts for Energy and Environmental Applications

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Abstract

Energy crisis and environmental deterioration has emerged as major problems around the world in recent times, mainly due to combustion of fossil fuels and their depletion. The utilization of light and thermal energy to produce chemical fuels is an attractive and major strategy to address the global energy crisis and other environmental issues. Our research group has recently developed several two-dimensional materials supported on nanostructured photocatalysts based on semiconductors, plasmonic materials, perovskite structures and upconversion nanoparticles for energy generation and environmental remediation applications. In addition to photocatalytic hydrogen generation, nitrogen fixation and pollutants degradation, our group has also utilized these materials for plastics upcycling, carbon dioxide conversion and Green organic transformations, either by functionalization or doping with a heteroatom. The highlights of the ongoing research work of our group in sustainable chemistry and heterogeneous catalysis will be presented.

References

1. S. Kumar, D. Sajwan, D. Sharma and V. Krishnan, *Adv. Sustainable Syst.* 2025, 9, 2500003.
2. D. Sharma, D. Sajwan, S. Mishra, A. Gouda, P. Mittal, P. Choudhary, B. P. Mishra, S. Kumar and V. Krishnan, *Nanoscale Horizons* 2025, 10, 423-459.
3. S. Kumar, P. Choudhary, D. Sharma, D. Sajwan, V. Kumar and V. Krishnan, *ChemSusChem* 2024, 17, e202400737.
4. D. Sajwan, A. Sharma, M. Sharma and V. Krishnan, *ACS Catal.* 2024, 14, 4865-4926.
5. S. Kumar, P. Choudhary, D. Sharma, D. Sajwan, V. Kumar and V. Krishnan, *ChemSusChem* 2024, 17, e202400737.
6. D. Sharma, P. Choudhary, P. Mittal, S. Kumar, A. Gouda and V. Krishnan, *ACS Catal.* 2024, 14, 4211-4248.
7. K. Kumari, P. Choudhary and V. Krishnan, *Catal. Sci. Tech.* 2024, 14, 5352 – 5363.
8. H. Chand, P. Bhumla, N. Allasia, G. Vile, S. Bhattacharya and V. Krishnan, *J. Colloid Interface Sci.* 2024, 673, 943-957.
9. D. Sharma, P. Choudhary, S. Kumar and V. Krishnan, *J. Colloid Interface Sci.* 2024, 657, 449-462.
10. H. Chand, A. Kumar, S. Goswami and V. Krishnan, *Fuel* 2024, 357, 129757

| KL-03 |

Reinforcing a Lithium-ion Battery Cathode (NCA) with Mn Doping

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Abstract

Nickel-rich layered oxide cathodes have emerged as one of the leaders for next-generation lithium-ion batteries (LIBs), offering high energy density and a relatively lower cobalt content. However, challenges such as cation mixing, structural degradation, and poor cycle retention persist. In this study, we systematically investigate the effect of controlled manganese (Mn) substitution in a NCA cathode materials synthesized via a solid-state route, targeting enhanced structural and electrochemical stability via manipulation of covalency of the material. XRD, Rietveld and TEM analyses confirm single-phase layered α -NaFeO₂-type structures with decreasing phase purity and increasing c/a ratios at high Mn content ($x \geq 0.2$), indicating an increased cation antisite disorder in the samples with increasing Mn contents. Mn introduction affects oxidation states of both Ni and Co leading to defects in the structure. Besides, due to Jahn-Teller distortion, particles undergo pulverization with the introduction of Mn. The presence of excess of Mn on the particle surface is confirmed with EELS. The sample with $x = 0.1$ (NMCA-1) demonstrated the optimal balance, exhibiting minimal lattice strain (0.0004%), the smallest crystallite size (~50 nm), structural integrity with an I(003)/I(104) ratio of 1.25 indicating minimal antisite disorder and enhanced thermal stability. Electrochemically, NMCA-1 delivered the highest capacity retention (~85% after 100 cycles at 0.2C), outperforming both undoped NCA (~70%) and fully Mn-substituted NMA (~45%). Despite a slight reduction in initial capacity (137 mAh g⁻¹), NMCA-1 exhibited superior rate capability (77 mAh g⁻¹ at 2C) and reduced overpotential growth, confirmed by CV and EIS analyses. Our findings highlight the synergistic effect of Mn and Al co-doping in optimizing cathode performance by tuning structural strain, mitigating phase degradation, and enhancing long-term cycling behaviour. This approach offers a cost-effective and scalable strategy to engineer high-performance cathode materials for future LIB applications.

References:

- (1) Wan, D. Y.; Fan, Z. Y.; Dong, Y. X.; Baasanjav, E.; Jun, H.-B.; Jin, B.; Jin, E. M.; Jeong, S. M. Effect of Metal (Mn, Ti) Doping on NCA Cathode Materials for Lithium Ion Batteries. *Journal of Nanomaterials* 2018, 2018, 1–9. <https://doi.org/10.1155/2018/8082502>.
- (2) Wang, B.; Zhang, F.; Zhou, X.; Wang, P.; Wang, J.; Ding, H.; Dong, H.; Liang, W.; Zhang, N.; Li, S. Which of the Nickel-Rich NCM and NCA Is Structurally Superior as a Cathode Material for Lithium-Ion Batteries? *J. Mater. Chem. A* 2021, 9 (23), 13540–13551. <https://doi.org/10.1039/D1TA01128F>

| KL-04 |

Molecular Crystals as New Materials for Photonic Circuits and Visible Light Communication

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Abstract

Recently, nano/micro-organic solids have emerged as promising materials for producing miniaturized organic photonic components, such as optical waveguides (active/passive), lasers, resonators (including chiral ones), filters, and modulators suitable for constructing organic photonic integrated circuits (OPICs).¹⁻³ Atomic force microscopy (AFM) is an effective technique to mechanically micromanipulate miniature organic photonic components towards OPICs - an approach known as *Mechanophotonics*. I will introduce examples of miniature organic photonic components fabricated from novel materials in my talk. I will also discuss the construction of OPICs with active, passive, and energy-transfer attributes using mechanophotonics. The fabricated OPICs switch, split, direct, and filter optical signals for signal enhancement, sensing, information processing and switchable photonic device applications. Recently, we have shown that text and image data can be transferred through fluorescent organic crystals for visible light communication at all angles.

References

1. R. Chandrasekar, *Small*, 2021, 17, 2100277.
2. R. Chandrasekar, *Chem. Commun.* 2022, 58, 3415-3428.
3. R. Chandrasekar et al. *Adv. Opt. Mater.* 2020, 8, 2000959.
4. M. Chosenyah, S. Rajaram, V. Novikov, A. Maydykovskiy, A. Khapre, T. Murzina, R. Chandrasekar, *J Am. Chem. Soc.*, 2026, Accepted.
5. M. Rohullah, V. Vinay Pradeep, S. Singh and R. Chandrasekar, *Nat. Commun.* 2024, 15, 4040.
6. A. V. Kumar, M. Rohullah, M Chosenyah, R. Chandrasekar, *Angew. Chem. Int. Ed.* 2025, 64, e202502122.
7. A. Khapre, J. Hazarika, R. Chandrasekar, *Nat. Commun.* 2025, 16, 10862.

| KL-05 |

Emerging Functions of Tröger's Base-Amino-1,8-Naphthalimides in Supramolecular Materials Design

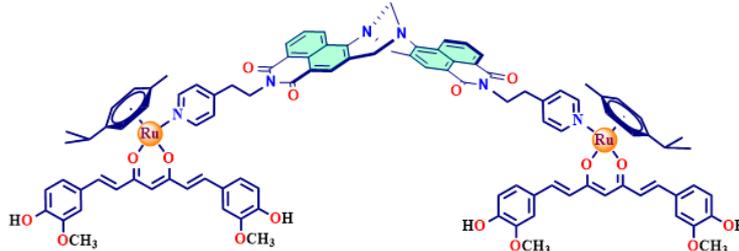
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Abstract

The design of functional supramolecular materials relies on the precise orchestration of noncovalent interactions to control molecular organization across multiple length scales. In this presentation, I will discuss our research on Tröger's Base-Amino-1,8-Naphthalimide (TBNap) derivatives as emerging supramolecular scaffolds for constructing hierarchically organized and responsive materials. The rigid, V-shaped and inherently chiral Tröger's base framework, when integrated with the highly emissive amino-1,8-naphthalimide fluorophore, offers a structurally defined and electronically tuneable platform for controlled self-assembly. We demonstrate how rational molecular design enables modulation of hydrogen bonding, π - π stacking, and host-guest interactions to direct aggregation in solution and solid states. Structural variation of substituents allows fine control over photophysical behaviour, including aggregation-induced emission enhancement and environment-sensitive fluorescence responses. These systems exhibit selective molecular recognition and stimuli-responsive properties, highlighting their potential in chemosensing and smart optical materials. The talk will emphasize structure-property relationships, mechanistic insights into self-assembly processes, and the translation of molecular design into functional material performance. Overall, TBNap-based architectures illustrate how thoughtfully engineered supramolecular scaffolds can bridge fundamental chemistry and advanced materials applications.



References:

1. M. K. Noushija, S. Hanson, D. Umadevi, N. Mishra, S. Shanmugaraju*. Chem. Asian J. 2026, 21, e70309.
2. M. K. Noushija, S. Shanmugaraju*. Anal. Sens. 2026, e202500165 (Advance Article).
3. S. Shanmugaraju*, D. Umadevi, A. J. Savyasachi, C. S. Hawes, J. A. Kitchen, G. J. McManus, T. Gunlaugsson*. Small Sci. 2025, 5, e202500386.
4. K. Balamurugan, M. Sandhiya, H. Gangadharan, M. K. Noushija, A. V. Krishna, A. Shanmughan, S. Shanmugaraju*. Ind. Eng. Chem. Res. 2025, 64, 23211.
5. Shanmughan, A.; Balamurugan, K.; Kalaiarasi, G.; Chitrarasu, K.; Shanmugaraju, S*. ACS Meas. Sci. Au., 2025, 5, 56.

| KL-06 |

Battery Electrodes: Nano vs Micro-Structuring

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Abstract

Battery electrodes comprise a current collector onto which a mix of active material particles, conductive carbon and binder additives are deposited. While this basic design has persisted for decades, the desired “size” of the active material particle is a matter of debate. Advances in nanotechnology have spurred interest in deploying nanoparticles as the active material. In this talk, I will compare nano with micro-particle electrodes, and discuss why the battery industry is unlikely to replace micro with nano-size particles. Given this, I will address the question as to whether there is a place for nanomaterials in battery design. I will show that the way forward lies in micro-particles constructed by the assembly of nanoscale building blocks and in micro-particles with engineered or natural nano-porosity. Such "multiscale particles" offer exciting possibilities to develop the next-generation of battery electrodes that are quintessentially both micro and nano with respect to their performance attributes.

Related publications

(1) Rishabh Jain, Aniruddha Singh Lakhnot, Kevin Bhimani, Shyam Sharma, Varad Mahajani, Reena A. Panchal, Mithil Kamble, Fudong Han, Chunsheng Wang, Nikhil Koratkar, "Battery Electrodes: Nano vs Micro-Structuring", NATURE REVIEWS MATERIALS 7, 736-746 (2022).

(2) A. S. Lakhnot, K. Bhimani, V. Mahajani, R. Panchal, S. Sharma, N. Koratkar, “Reversible and Rapid Calcium Intercalation into Molybdenum Vanadium Oxides”, PNAS 119, e2205762119 (2022).

| KL-07 |

Metal-free Electrocatalysts: Defects vs Heteroatom(s)

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Abstract

Since the inception of cobalt phthalocyanine for oxygen reduction reaction (ORR), non-platinum group metals have been the central focus in the area of fuel cell electrocatalysts. Metal-free carbon catalysts stand out for their durability in the air cathodes of the metal-air batteries. Understanding the origin of the active sites in the heteroatom-doped carbon material plays a vital role in designing novel electrocatalysts for the ORR in fuel cell cathodes. In this seminar, the effect of carbon defects vs heteroatom(s) is discussed. The topological and edge defect contributions to the ORR activity are studied using chemical functionalization and intentionally created edge defects via the mechanochemical process. Mainly, the boron and nitrogen-doped carbon materials are analysed for their ORR activity. Our studies have tried to separate the contribution of each active site to the overall ORR activity of the multi-heteroatom-doped carbon materials.

ORAL PRESENTATIONS

| OP-01 |

From Sustainable Materials to Human Health: Rethinking Air Pollution Mitigation through Interdisciplinary Chemistry

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Abstract

Air pollution remains one of the most pervasive environmental challenges, affecting human health across respiratory, cardiovascular, and neurological systems. While material chemistry has delivered significant advances in pollutant capture, filtration, and remediation, translation of these innovations into meaningful health outcomes remains limited. This gap arises largely from the fragmented way in which materials science, environmental chemistry, and health sciences operate. This talk will present air pollution as a multiscale challenge, where molecular-level material design must be aligned with exposure pathways, physiological responses, and real-world deployment constraints. Using examples from sustainable and functional materials, the discussion will highlight how material properties such as surface chemistry, porosity, biodegradability, and scalability influence not only pollutant removal efficiency but also human exposure reduction and downstream health relevance. Rather than focusing on specific devices or datasets, the presentation will emphasize conceptual frameworks for integrating materials chemistry with biological and physiological endpoints. Key opportunities and unmet needs at the materials–health interface will be discussed, including the importance of interdisciplinary collaboration for designing solutions that are affordable, scalable, and health-relevant. By reframing air pollution mitigation as a shared challenge between chemists, materials scientists, and life scientists, this talk aims to stimulate cross-disciplinary dialogue and identify pathways where sustainable chemistry can contribute more directly to improving air quality and human well-being.

Keywords: Air pollution, Sustainable materials, Human health, material and Environmental chemistry

| OP-02 |

Dual-Function Modified g-C₃N₅ Nanodots for Ultra-Sensitive Luminescent Detection and Complete Degradation of Ciprofloxacin

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Abstract

The widespread use of antibiotics has resulted in their continuous presence in aquatic environments, raising critical ecological and human health concerns. Herein, we present a dual-functional strategy employing graphitic carbon nitride (g-C₃N₅) nanodots (g-CND) synthesized via ultrasound-assisted thermal polycondensation for the luminescent sensing and photocatalytic degradation of ciprofloxacin (CPFX). The g-CND demonstrated exceptional sensitivity and selectivity for CPFX detection, achieving an ultra-low detection limit of 0.13 nM through fluorescence quenching. Following detection, the g-CND based heterojunction enabled efficient photocatalytic degradation of CPFX under visible light, exhibiting degradation efficiency of 98%. The material revealed remarkable stability, retaining its degradation performance over multiple cycles. This comprehensive approach not only allows rapid and accurate detection of antibiotics but also provides an effective means for their removal from water, highlighting the potential as a cost-effective and sustainable solution for real-time monitoring and treatment of antibiotic residues in aquatic environments.

Keywords: g-CND, Ciprofloxacin, Luminescent sensor, Photocatalytic Degradation, Water treatment

| OP-03 |

Hesperetin:4-Aminopyridine Cocrystal (2HSRT:4AP)-A Strategy for Improving Solubility

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Abstract

Hesperetin (HSRT) is a weak acidic flavonoid with low aqueous solubility and is mainly found in citrus fruits. It is also reported to have various biological properties, including antioxidant, anti-inflammatory, anti-cardiovascular, and chemopreventive effects. Despite its therapeutic potential, HSRT is classified as a Class II flavonoid according to the Biopharmaceutical Classification System (BCS) due to its higher permeability and low solubility. To enhance the aqueous solubility of HSRT, a crystal engineering strategy is employed in this work to obtain a favorable solid form of HSRT with various coformers, without altering its pharmacological activity. Among various coformers tested with HSRT, 4-Aminopyridine (4AP) was found to bind with HSRT and produce a neutral cocrystal (2HSRT:4AP) in a 2:1 ratio using the slow evaporation method. The 2HSRT:4AP cocrystal was examined in this work using structural characterization (SCXRD, PXRD, FT-IR) and thermal analysis (DSC and TGA). The SCXRD studies revealed that the cocrystal is stabilized by an intermolecular N-H \cdots O hydrogen bonding interaction in the supramolecular framework. Equilibrium solubility study using the shake-flask method demonstrated that the solubility of HSRT has been significantly enhanced upon cocrystallization. Geometry optimization of the cocrystal was performed using DFT at the ω B97XD/6-311++G(d,p) level, followed by vibrational frequency calculations to compare simulated and experimental FT-IR spectra. NBO analysis was performed to elucidate inter- and intramolecular hydrogen-bonding interactions involved in cocrystal formation. To further validate the supramolecular assembly of the cocrystal in the crystalline lattice, Hirshfeld surface analysis was performed, and the predominant interactions in the crystalline lattice were identified using fingerprint plots.

Keywords: Pharmaceutical cocrystals, Supramolecular synthon, Cocrystallization, Molecular interactions, Equilibrium solubility

| OP-04 |

Supramolecular Crystal Engineering Approach for Assembling 18-Crown-6 Ether ($C_{12}H_{24}O_6$) 4-Aminopyridinium Perchlorate Complex ($C_5N_2H_3^+.ClO_4^-$) for Nonlinear Optical Applications

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Abstract

The exploration of Nonlinear optical (NLO) crystalline materials has fascinated numerous researchers owing to their widespread applications in the fields of optoelectronics, photonic devices and laser technology. Supramolecular crystal engineering, especially host-guest encapsulation of Crown ethers, has gained attraction due to their structural stability, favourable charge transfer characteristics leading to NLO response. Here, we introduce a new class of organic-inorganic supramolecular complex compound, 18-crown-6 with 4-aminopyridinium perchlorate, synthesised as single crystals using the slow evaporation technique. The crystal structure was elucidated by single-crystal X-ray diffraction, revealing that the complex crystallises in the centrosymmetric space group P-1, and the complex is stabilised by intermolecular interactions through $N^+ \cdots H \cdots O$. The vibrational characteristics were analysed using FT-IR and Raman spectroscopy, which confirms the presence of functional groups within the complex. Meanwhile, the UV-Vis analysis showed a wider transparency region from 300 to 800 nm, with an optical band gap of 4.3 eV. The nonlinear refractive index and optical limiting threshold of the complex were obtained using Z-scan studies. Hirshfeld analysis provided insights into the intermolecular interactions within the complex, and their dominant interactions were identified using 2D fingerprint plots. Hence, these results indicate that the titled supramolecular crystal is a suitable candidate for NLO applications.

Keywords: Crown-ether complex, Supramolecular chemistry, Z-scan, Nonlinear optical applications, Hirshfeld analysis

| OP-05 |

Mononuclear Palladium(II) Hydrazone Complex: Synthesis, Characterization and *In Vitro* Cytotoxicity towards Human Cancer Cells

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Abstract

Palladium(II) complex [Pd(L)(PPh₃)] was synthesized using a mono dentate dibasic hydrazone ligand (HL). Synthesized complex was characterized by spectroscopic and single crystal XRD analysis. From the single crystal XRD analysis, distorted square planar geometry of the palladium(II) complex was confirmed. The cytotoxicity of the ligand and complex was examined against MDA-MB-231 human breast cancer cell. The results revealed that the complex exhibit a higher activity than its corresponding ligand. The growth study of MDA-MB-231 breast cancer cells carried with ligand and Pd(II) complex, the cell toxicity of complex is more when compared with ligand. Further, AO/PI staining assay was carried to identify the mode of cell death, and the results demonstrated that the complex exhibited significant activity in inducing cell death than the ligand activity against the MDA-MB-231 cell line. The results revealed that the proposed complexes exert cytotoxic effects by inducing apoptosis.

Key words: Palladium complex, Mono-dentate dibasic hydrazone, MDA-MB-231, Human Breast Cancer cell, AO/PI staining assay.

| OP-06 |

Uniform Coating of NiO-Nanoparticles on Diamond Particles as Efficient and Stable Catalyst for Hydrogenation of Carbonyl Compounds

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Abstract

Highly active and cost-effective metal nanoparticle (NiO) supported diamond particle (DP) nanocomposite (NiO-DP) were prepared by sonochemical method for hydrogenation of carbonyl compounds. The strong interfacial interaction between NiO and diamond nanoparticles significantly modified the optical and structural properties of NiO. The HR-TEM images showed the uniform dispersion of metal particle on diamond surfaces. The metal nanocomposite was characterized by UV-Vis, IR, XRD, SEM and EDX. The significant metal-diamond interaction was studied by means of X-ray photoelectron spectroscopy (XPS). The catalytic efficiency of NiO-DP was evaluated for hydrogenation reaction which shows significant efficiency. The catalyst exhibits an excellent stability and recyclability without loss of activity. The synergistic effect between NiO and diamond nanoparticles enhanced electron transport, active site accessibility, and surface reactivity.

Keywords: Nanostructured materials, Nickel oxide (NiO), Diamond nanoparticles (DNP), Nanocomposites, Hydrogenation, Catalysis.

|OP-07|

Peripherally Fluorinated Tetraphenylethene: New Electron Extraction Interlayers for n-i-p Perovskite Solar Cells

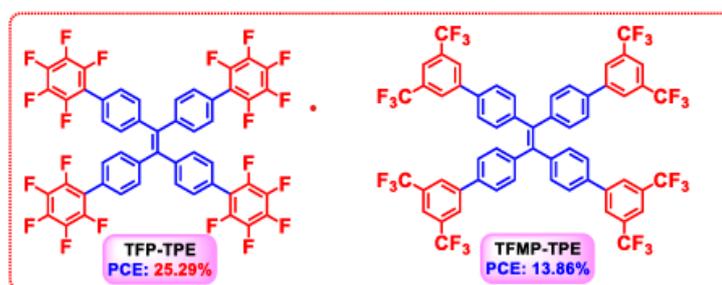
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Abstract

Tetraphenylethene (TPE) is a widely used structural motif in optoelectronic materials due to its high structural versatility. However, conventional TPE-based interlayers in perovskite solar cells (PSCs) often suffer from poor interfacial compatibility, leading to inefficient charge extraction and limited device stability. To address these challenges, we designed two fluorinated TPE-based electron-transporting interfacial materials by introducing hydrophobic phenyl substituents: 1,1,2,2-tetrakis(2',3',4',5',6' pentafluoro-[1,1'-biphenyl]-4-yl)ethene (TFP-TPE, 1) and 1,1,2,2-tetrakis(3',5'-bis(trifluoromethyl)-[1,1' biphenyl]-4-yl)ethene (TFMP-TPE, 2). Single-crystal X-ray diffraction reveals highly twisted molecular conformations, which suppress aggregation and improve film uniformity. These fluorinated interlayers enhance surface wettability, strengthen interactions with perovskite precursors, and regulate crystallization dynamics, resulting in improved interfacial quality and more efficient charge collection. Photoluminescence studies confirm enhanced electron extraction and transport, particularly for TFP-TPE. PSCs incorporating TFP-TPE achieve a highpower conversion efficiency of 25.29%, among the best reported for organic interfacial materials. Moreover, the devices exhibit excellent stability under high humidity and elevated temperatures. This work demonstrates a simple and effective molecular design strategy for high performance and stable PSCs, highlighting the critical role of hydrophobic fluorinated interfaces.



Keywords: Photoluminescence, Optoelectronic, Perovskite

| OP-08 |

An ESIPT-Active TREN-1,8-Naphthalimide Schiff Base Fluorescent Probe for Selective Zn(II) Sensing and Bioimaging

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Abstract

Zinc plays a crucial role in biological processes and environmental systems¹; however, its abnormal levels are associated with serious health disorders and ecological risks. Rapid, selective, and low-toxicity detection of Zn(II) is therefore essential for environmental monitoring and biological diagnostics.^{2,3} In this study, we report a TREN-1,8-naphthalimide-based Schiff base fluorescent probe, **NapSB**, designed for practical Zn(II) sensing applications. **NapSB** was synthesised via a simple one-pot strategy and fully characterised by spectroscopic techniques and single-crystal X-ray diffraction. The probe exhibits a strong and selective fluorescence response toward Zn(II) through an excited-state intramolecular proton transfer (ESIPT) mechanism, enabling sensitive detection with a limit of 5.85 ppm even in the presence of competing metal ions. Importantly, **NapSB** demonstrates reliable performance in real water samples, highlighting its potential for environmental zinc monitoring. Furthermore, cellular imaging studies reveal significant fluorescence enhancement upon Zn(II) binding, confirming efficient cell permeability and selective intracellular Zn(II) detection. Owing to its synthetic simplicity, high selectivity, and dual environmental-biological applicability, **NapSB** represents a promising fluorescent platform for practical zinc sensing and bioimaging applications.

Keywords: Zinc(II) sensing, Fluorescent probe, ESIPT mechanism, Bioimaging, Environmental monitoring

| OP-09 |

Tröger's Base Containing N-Rich Porous Metal-Organic Frameworks for Selective and Enhanced Adsorption of CO₂

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Abstract

Nitrogen-rich metal-organic frameworks (MOFs) have emerged as promising materials for CO₂ sorption and storage because of their strong Lewis-basic N-sites, tuneable pore environments, and ability to engage in favourable dipole-quadrupole interactions with CO₂.¹ Incorporating N-donor functionalities into MOF linkers enhances binding affinity, selectivity, and adsorption capacity, particularly under ambient conditions relevant to post-combustion carbon capture. In this work, a 4-amino-1,8-naphthalimide-derived Tröger's base linker was synthesized and employed to construct nitrogen-rich MOFs for selective CO₂ adsorption. The rigid, V-shaped Tröger's base core provides structural robustness, intrinsic fluorescence, and multiple Lewis-basic sites that promote strong CO₂ interactions. The resulting MOF exhibit high porosity, tuneable pore architectures, and enhanced host-guest interactions arising from abundant nitrogen donors. Gas-sorption studies reveal significantly improved CO₂ uptake and CO₂/N₂ selectivity under ambient conditions. These findings underscore the potential of Tröger's base-based linkers in advancing next-generation porous materials for efficient carbon-capture applications.

Keywords: Tröger's base, Metal-organic frameworks, Naphthalic anhydride, Naphthalimide

| OP-10 |

Gd-Doped NiWO₄ Heterostructures with ZnO and ZnSe for Enhanced Charge Transport and Electrocatalysis

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Abstract

The increasing demand for sustainable energy technologies has intensified research on multifunctional electrode materials capable of efficient energy storage and electrocatalytic performance. Nickel tungstate (NiWO₄) is a promising transition metal oxide due to its chemical stability and redox activity; however, its moderate electrical conductivity and sluggish charge transfer limit practical applications. To address these issues, electronic structure modulation and interfacial engineering are required. In this study, pristine NiWO₄, gadolinium-doped NiWO₄, and heterostructured ZnO/Gd/NiWO₄ and ZnSe/Gd/NiWO₄ composites were synthesized via a facile hydrothermal method, enabling controlled crystal growth, uniform dopant incorporation, and strong interfacial coupling. Gd doping introduces lattice defects that modify the electronic structure, while ZnO and ZnSe coupling forms heterojunctions that promote efficient charge separation and transport. Structural and optical analyses confirmed the formation of phase-pure materials and well-integrated heterostructures. UV-Vis diffuse reflectance spectroscopy showed that the band gap of pristine NiWO₄ (2.54 eV) decreases to 1.85 eV after Gd incorporation, whereas heterostructure formation increases the band gap to 2.80 eV for ZnO/Gd/NiWO₄ and 3.18 eV for ZnSe/Gd/NiWO₄ due to strong interfacial interactions. Electrochemical studies reveal that Gd doping enhances conductivity and redox activity, while heterostructuring further improves electron transport and electroactive surface area. Among all samples, ZnSe/Gd/NiWO₄ exhibits the highest specific capacitance, good rate capability, excellent cycling stability, and reduced overpotentials for both hydrogen and oxygen evolution reactions, highlighting its potential for supercapacitor and water-splitting applications.

Keywords: Nickel tungstate, Heterostructures, Band gap engineering, Supercapacitors, Electrocatalysis, Water splitting, Zinc selenide, Zinc oxide

| OP-11 |

Synergistic Heterointerface Engineering of $\text{Ti}_3\text{C}_2\text{T}_x/\text{g}-\text{C}_3\text{N}_4$ Bilayers for Robust Sn-Based Alloying-Type Negatrodes for Sodium-ion Pouch Batteries

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Abstract

In this work, a $\text{Ti}_3\text{C}_2\text{T}_x/\text{g}-\text{C}_3\text{N}_4$ bilayer hybrid composite containing tin nanostructures is developed for use as a high-performance anode material in sodium-ion pouch batteries. Initially, $\text{Ti}_3\text{C}_2\text{T}_x/\text{g}-\text{C}_3\text{N}_4$ bilayer hybrids with varying $\text{Ti}_3\text{C}_2\text{T}_x$ and $\text{g}-\text{C}_3\text{N}_4$ ratios are optimized to obtain a stable, porous matrix, which are subsequently used to support Sn nanostructures. As a result, a homogeneous Sn distribution within a conductive $\text{Ti}_3\text{C}_2\text{T}_x$ scaffold and nitrogen-rich $\text{g}-\text{C}_3\text{N}_4$ framework is achieved. Structural and surface analyses confirm the formation of the robust bilayer hybrid heterostructure with effective Sn nanostructure dispersion and strong interfacial interactions. The final $\text{Sn}@\text{Ti}_3\text{C}_2\text{T}_x/\text{g}-\text{C}_3\text{N}_4$ bilayer hybrid nanocomposite negatrode delivers a reversible capacity of $511 \text{ mAh}\cdot\text{g}^{-1}$ (0.5 C) with ~93% retention over 1000 cycles in half pouch cell format. Combined with a Ni-hexacyanoferrate positrode, the resulting full pouch cell delivers a reversible capacity of $61 \text{ mAh}\cdot\text{g}^{-1}$ (total mass, 0.5 C) translating to $192 \text{ Wh}\cdot\text{kg}^{-1}$ energy density with ~89% retention (1000 cycles).

Keywords: $\text{Ti}_3\text{C}_2\text{T}_x$, $\text{g}-\text{C}_3\text{N}_4$, Tin (Sn), Alloying-type, Negatrode, Sodium ion battery pouch

| OP-12 |

Computational Multi-Target Drug Discovery Pipeline for Diabetic Foot Ulcer Targeting VEGFR2, MMP-2/9, NF- κ B, and IL-1 β

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Abstract

Diabetic foot ulcers (DFUs) are a major complication of diabetes mellitus, characterised by chronic inflammation, impaired angiogenesis, extracellular matrix (ECM) degradation, and delayed tissue repair. Conventional therapies often fail due to the multifactorial and redundant nature of the underlying molecular pathways. Key pathological mediators include VEGFR2, MMP-2, MMP-9, NF- κ B, and IL-1 β , which collectively regulate angiogenesis, inflammation, and matrix remodelling. Targeting these pathways through the multi-target therapeutic strategy significantly improves wound healing activity and angiogenesis. The Current study utilises an integrated in silico drug discovery approach for the identification of novel small molecules with the capability of simultaneous activation of VEGFR2 and inhibition of MMP-2, MMP-9, NF- κ B, and IL-1 β . Crystal structures were retrieved from the RCSB Protein Data Bank and prepared in Schrödinger Maestro. Receptor–ligand pharmacophore models were generated using Phase with quercetin as the reference to define key interaction features. A curated library of 2000 small molecules from ChEMBL and PubChem was processed with LigPrep and filtered using QikProp for drug-likeness and ADMET properties. Hierarchical Glide screening (HTVS, SP, XP) identified top multi-target candidates with high predicted affinity, showing docking scores of \sim -8.0 to -11.2 kcal/mol across targets. Density Functional Theory analysis indicated favourable reactivity and stability, with HOMO–LUMO energy gaps in the optimal range (\sim 2.3–4.8 eV). Molecular dynamics simulations (200 ns) confirmed stable protein–ligand complexes with RMSD \sim 1.5–3.0 Å and persistent key interactions. Selected multi-target leads were advanced as topical gel candidates, showing potential to promote angiogenesis, reduce inflammation, limit ECM degradation, and accelerate diabetic wound healing.

Keywords: Diabetic foot ulcer, Multi-target approach, Pharmacophore modelling, Angiogenesis

| OP-13 |

An Artificial Intelligence-Powered Prediction and Optimization of Biogas Yield from Agro-Residues for Sustainable Energy

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Abstract

If agricultural waste is not managed, it contributes to greenhouse gas emissions and environmental pollution. Such biomass can be converted into biogas, which provides a sustainable way to generate renewable energy. In this project, a variety of agricultural residues, including sugarcane residue, manure, fruit peel, vegetable waste, grass clippings, corn stalks, wheat straw, and rice husk, will be applied to predict biogas production using machine learning techniques. To identify trends affecting methane production, a dataset of 5,000 records was preprocessed by waste type and examined. To determine the most accurate predictive method, several machine learning models were evaluated, including RF, Gradient Boosting, and Support Vector Regression. According to experimental results, rice husk and wheat straw yield lower yields than fruit peel and grass clippings, which suggests the need for pre-treatment techniques to increase efficiency. The created model provides researchers, policymakers, and biogas plant operators with an intelligent decision-support tool to enhance energy recovery, improve feedstock selection, and promote a circular economy. This work demonstrates how clean energy solutions derived from agricultural waste can be adopted more rapidly.

Keywords: Methane prediction, Biogas, Renewable energy, Agricultural waste, Machine learning, Sustainable energy

| OP-14 |

Negative Electrode for Next Generation Energy Storage Device

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Abstract

Metal chalcogenide -based anode shows significant promise as next generation electrode material in the field of rechargeable batteries. Layered structure, tunable band gap & better ion diffusion mechanism prompt them to have high specific capacitance, adequate power density with morphological modification makes these materials to achieve better rate capability than conventional anodes. This particular study focuses on developing novel anode material deviating from conventional graphite -based material which has been the most stable negative electrode for decades with 375 mAh/g (LiC₆) theoretical specific capacity and adequate conductivity. It is prone to dendrite formation, capacity fading and uncertain lifecycle due to pulverization and many issues come along. Thus, it has been in the focus of several research groups to look beyond anode material based on graphite and focus on advanced functional materials such as metal chalcogenide that promises higher specific capacity, multiple ion storing mechanism and are efficient in delivering the power. In the present study, we focus on tin based anode, which can store 4 lithium atoms per single tin atom with intermetallic alloying reaction, in comparison to 1 Li atom for 1 carbon atom in an intercalation mechanism in traditional graphite anode. Therefore, tin theoretically becomes a better choice for advanced material design for energy storage. Selection of sulphur among other chalcogenide enhances the electrode by improving the ion diffusion ability at negative electrode due to surface oxygen vacancy, non-toxicity and available abundantly it supports the economic aspect as well. Even though metal chalcogenide-based anode face issues such volume expansion, low conductivity with advanced morphological modification, adding titanium as a dopant enhances the conductivity and give the material structural strength to withstand the volume expansion.

Keywords: Anode, Chalcogenides, Hydrothermal method, Specific capacity

| OP-15 |

Design and Thermal Performance of Imidazole-Functional Benzoxazine/Epoxy Hybrid Polymer Networks

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Abstract

Benzoxazines are a class of thermosetting resins formed from the reaction of phenols, amines, and formaldehyde. They offer high thermal stability, low water absorption, excellent dimensional stability, and near-zero shrinkage upon curing. Their unique structure allows for tunable properties through monomer design, and they can be blended with epoxies or other resins to produce hybrid materials with enhanced mechanical, thermal, and flame-resistant performance. Benzoxazine monomers containing an imidazole core were synthesized and blended with epoxy resins to develop hybrid thermosets. The presence of the imidazole functionality facilitated efficient crosslinking at lower temperatures, resulting in well-formed networks. Thermal analysis showed that the hybrids exhibit enhanced thermal stability, high decomposition temperatures, and improved char formation compared to conventional systems. These findings demonstrate the potential of imidazole-containing benzoxazine/epoxy blends for applications requiring thermally stable and dimensionally reliable polymer networks.

Keywords: Imidazole, Benzoxazine/epoxy blend, Thermal stability.

| OP-16 |

A Naphthyl-Based Turn-on Fluorescent Chemosensor for Dual Detection of Ba²⁺ Ions and Mancozeb

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Abstract

The development of simple and sensitive sensing systems for environmentally hazardous species is of growing importance. Fluorescent chemosensors have emerged as powerful analytical tools due to their high sensitivity, operational simplicity, rapid signal generation, and capability for real-time monitoring. Barium ions (Ba²⁺), widely used in industrial and medical applications, can pose environmental and health risks upon excessive exposure. In addition, the extensive agricultural use of the fungicide Mancozeb leads to residue accumulation in soil and water, creating further ecological concerns. These issues demand rapid, reliable, and cost-effective detection strategies. In this work, a naphthyl-based fluorescent chemosensor **HNDB**, was developed as a multifunctional probe for the detection of Ba²⁺ ions and Mancozeb (MNZ). The probe exhibits weak intrinsic fluorescence, which undergoes a significant enhancement in the presence of Ba²⁺ and MNZ, producing a clear fluorescence “turn-on” signal. The sensor demonstrated high selectivity toward Ba²⁺ over various competing metal ions in DMF–H₂O (1:1) HEPES buffer medium at pH 7.3. Spectroscopic investigations and Job’s plot analysis confirmed stable complex formation. The probe HNDB also showed rapid response, good reproducibility, and stable performance across a broad pH range. These results demonstrate that **HNDB** serves as an efficient fluorescence-based platform for monitoring both metal ions and pesticide contaminants in environmental samples.

Keywords: Fluorescent chemosensor, Naphthyl, Ba²⁺ ion, Mancozeb

| OP-17 |

Design of a Uryl-Based Chemosensor for Dual Colorimetric and Fluorimetric Detection of Toxic Hg²⁺ Ions and Amino Acids

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Abstract

Fluorescent chemosensor have gained considerable attention in supramolecular chemistry due to their straightforward design, high sensitivity, and strong selectivity. Although these sensors were originally developed for detecting ionic and neutral species, they are now widely utilized in fields such as biological sciences, medicine, pharmacology, and environmental analysis. Among heavy metal ions, mercury is particularly concerning because it serves no beneficial biological role and is widely known for its severe toxicity. Prolonged exposure to mercury can lead to serious health issues, especially affecting the skin and eyes. Despite these risks, mercury continues to be extensively employed in dental composites, batteries, electronic components, and in metallurgical processes such as the extraction of gold and silver via amalgamation. In addition, the fluorescent properties of the developed probe enable the detection of aspartic acid. While aspartic acid is generally regarded as safe, excessive consumption may cause adverse effects, including liver dysfunction and gastrointestinal disorders. This study reports the synthesis and comprehensive characterization of a uryl-derived fluorescent chemosensor (ITC), engineered for the selective detection of Hg²⁺ ions using a colorimetric method and aspartic acid through fluorescence sensing. Investigations performed in a CH₃CN₂O (1:1) buffered medium at physiological pH (7.4) demonstrated a pronounced red shift in the optical response for both detection mechanisms, confirming the probe's efficiency and selectivity toward Hg²⁺ ions and aspartic acid under biologically and industrially relevant conditions.

Keywords: Chemosensor, Uryl, Heavy metal ion, Mercury, Aspartic acid

| OP-18 |

Mono Nano-Probe, Duo Signals: Dual Colorimetric And Fluorescent Detection of Dimethoate and Chlorpyrifos

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Abstract

Fluorescent chemosensors are specialized molecular systems that detect target analyte through fluorescence signal changes. Fluorescent chemosensors incorporated with Nano-probes have provoked significant amount of interest in forensic science, particularly for the detection of pesticides due to their exceptional sensitivity, rapid response and ability to function in complex sample matrices such as blood, saliva, soil and food. Pesticides are chemical substances widely employed in agriculture to control pests and increase crop productivity. Despite their agricultural benefits these compounds possess varying degree of acute and chronic toxicity which pose serious health risk when improperly used or intentionally misused. In recent times, pesticide poisoning has gained much more forensic importance due to their frequent involvement in suicidal, accidental and homicidal poisoning cases. The easy accessibility, low cost and high lethality of pesticides especially organophosphates and carbamates are frequently involved in poisoning cases and have made them common agents of concern in forensic toxicology. In this study, a Nickel oxide (NiO) based Fluorescent Nano Probe (FNP) has been developed and utilized as a fluorescent chemosensor, tailored for the dual detection of organophosphorous pesticide, chlorpyrifos residues in photoluminescence spectroscopy and on the other hand it aids for the colorimetric detection of dimethoate pesticide in forensic matrices. In aqueous medium, the nano probe with the targeted analyte have exhibited distinctive peak which laid the groundwork and achieved detection through fluorescence and UV-VIS spectroscopic signaling with high selectivity and low sensitivity.

Keywords: Nano probes, Pesticide detection, Fluorescent chemosensors, Organophosphates, Fluorescence signaling

| OP-19 |

Temperature-Dependent Lattice Dynamics of Barium Zirconate Using First-Principles Quasi-Harmonic Phonon Calculations

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Abstract

We investigate the temperature-dependent structural and thermodynamic properties of barium zirconate using density functional theory combined with quasi-harmonic phonon calculations. Phonon dispersions, vibrational free energies, and equilibrium volumes are computed over a broad temperature range to quantify thermal effects on the lattice. With increasing temperature, a systematic softening of phonon modes is observed across the spectrum, accompanied by progressive elongation of Ba-O and O-O bonds. Vibrational enthalpy and entropy contributions further indicate enhanced lattice relaxation, leading to increased thermodynamic stability at elevated temperatures. The calculated bulk modulus and thermal expansion coefficients are in good agreement with experimental measurements. These results demonstrate the central role of vibrational contributions in governing lattice stability and provide microscopic insight relevant to high-temperature electrochemical applications.

Keywords: Quasi-harmonic approximation, Phonon calculations, Density functional theory, Thermal expansion

| OP-20 |

2D Amphiphilic Janus silica from natural clay as sustainable Pickering emulsifier

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Abstract

Pickering emulsifiers are solid particles that facilitate superior stabilization of emulsions against coalescence than molecular surfactants. Amphiphilic Janus particles represent a class of carefully designed particles with spatially segregated hydrophilic and hydrophobic surfaces. Their intermediate wettability and self assembling behaviour make them ideal choice for durable emulsification performance. However, there exist challenges in the scalability, cost and sustainability aspects which limit their application in food, cosmetic and pharmaceutical industries. In the current work, montmorillonite, a 2D aluminosilicate clay is modified into amphiphilic Janus sheets using ultrasonication to exfoliate clay followed by Pickering emulsion template method for partial silanization of exfoliated nanosheets. Effect of electrolyte concentration on the formation of silica sheet-stabilized wax-in-water emulsion is studied. Field Emission Scanning Electron Microscopic images provide evidence on the formation of silica sheet-stabilized wax microspheres where one side of the sheet is masked under solidified wax. The amphiphilic silica sheets showed intermediate surface contact angle in comparison to its isotropic hydrophilic and hydrophobic counterparts. The degree of silanization from thermogram analysis revealed mid percentage mass loss and partial degree of functionalization relative to its counterparts. The *in vivo Allium cepa* root tip assay showed negligible cytotoxicity of 2D silica sheets on meristematic cells. The clay-based Janus silica sheets showed spontaneous assembling at the oil-water interface and upon ultrasonication produced stable emulsion. The Janus particles retained more than 50 % emulsification index with 25 μm droplet size distribution after 24 h. Therefore, the present work describes the sustainable conversion and utilization of natural clay as potential emulsifiers.

Keywords: Montmorillonite, silica, Amphiphilic Janus, Pickering emulsion, *Allium cepa* root tip assay

| OP-21 |

Super Capacitors the Future for Energy Storage

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Abstract

In recent years, globe facing so many social issues, and looking for the better life standard, through the innovative green technologies. In Day-to-day life humans' society is in major energy needs increases as population increases. Also, researchers are finding alternate energy resources like solar energy, wind energy, geothermal energy etc., it is giving solution to the problem of pollution (Water, Air, Land, Soil pollutions). Carbon di-oxide emissions nowadays increases and it cause global warming. To resolve this problem, we need alternate energy resources for fossil fuels. Supercapacitors are the most valid innovation in the field of Energy storage. Super Capacitors have become more and more popular because of their great cycle stability and high-power density. The nanocomposite materials were synthesised using hydrothermal synthesis methods. The rare earth metal tungstate was combined with transition metal oxides, sulphides, phosphates etc., The synthesized compounds were coated in a suitable coating surface like reduced graphene (rGO). The nanocomposites are characterized using XRD, IR, UV, SEM-EDX, TEM, XPS to analyse the morphological studies of synthesised nanoparticles and biological studies. The electrocatalytic properties of the nanoparticles were then investigated using cyclic voltammetry and electrochemical impedance spectroscopy. This study introduces a new approach to the chemistry of materials and the environment and demonstrate that a careful selection of components can lead to a new horizon of material science.

Keywords: Supercapacitors, Energy storage device, Nanocomposites, Fossil fuels, Zero pollution.

| OP-22 |

Interfacial Design of 1T-MoS₂/Co₃O₄ Composite for Enhanced Electrocatalytic Oxygen Evolution Reaction

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Abstract

The development of efficient and durable electrocatalysts for the oxygen evolution reaction (OER) is essential for improving the activity and durability of electrochemical energy conversion technologies. Transition metal dichalcogenides (TMDs) are becoming potential electrocatalysts due to their unique electronic properties, layered structure, and natural abundance. Practically, their performance is limited by their low intrinsic conductivity and the confined nature of the active sites. Various strategies are employed to enhance their conductivity and create more active sites, thereby achieving improved catalytic activity. In addition, transition metal oxides (TMOs) exhibit a mixed-valence state, containing both 2+ and 3+ metal ions. This distinct arrangement improves its catalytic performance for OER. In this work, a 1T-MoS₂/Co₃O₄ composite electrocatalyst was synthesized and evaluated for OER performance. The 1T-MoS₂/Co₃O₄ electrode exhibits a significantly lower overpotential, a smaller Tafel slope, and better catalytic activity compared to pure 1T-MoS₂ and Co₃O₄ in 1M KOH. The combination of metallic 1T-MoS₂ with Co₃O₄ enhances electrical conductivity, increases the active sites, and promotes charge transfer across the interface between 1T-MoS₂ and Co₃O₄. The 1T-MoS₂/Co₃O₄ catalyst shows long-term stability even after 5000 cycles. The i-t curves measurement shows minimum degradation and better durability, confirming the stability of the 1T-MoS₂/Co₃O₄ in OER. These results highlight the 1T-MoS₂/Co₃O₄ composite as an alternative to noble metal electrocatalysts for efficient OER. Keywords: TMDs, Co₃O₄, Electrocatalyst, Oxygen evolution reaction.

Keywords: Electrocatalysts, Transition metal dichalcogenides, OER.

| OP-23 |

Cascade Synthetic Strategy Toward Novel Triazoles: SAR Analysis and Molecular Modeling Insights

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Abstract

A cascade synthetic strategy was developed for the efficient synthesis of structurally diverse and novel triazole derivatives (**Fig.1**). The protocol enables rapid molecular complexity generation under environmentally benign conditions with excellent yields. The synthesized compounds were fully characterized using spectroscopic techniques. Biological evaluation of the triazole derivatives revealed notable activity, and structure–activity relationship (SAR) analysis highlighted the critical role of substituent type and position on the triazole scaffold. Molecular modeling studies were performed to rationalize the observed SAR trends, demonstrating favorable binding orientations and key interactions with the selected biological target. The combined experimental and computational results provide valuable insights into the design and optimization of novel triazole-based bioactive scaffolds.

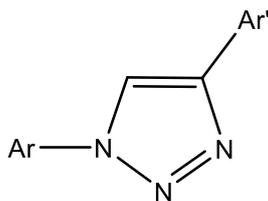


Fig. 1

Keywords: Triazole, Molecular modelling, SAR

| OP-24 |

Magnesium Salt-Doped Pectin/Guar Gum Electrolytes: A Bio-Based Approach to Energy Storage Materials

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Abstract

Concerns over the environmental impact of conventional energy storage devices such as issues of sustainability, non-biodegradability, and toxicity have driven the pursuit of eco-friendly biopolymer electrolytes. In this work, blended biopolymer electrolytes were synthesized using a pectin/guar gum (PG) blend as the polymer host, magnesium chloride hexahydrate ($\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$) as the ionic dopant, and succinonitrile (SN) as a plasticizer, prepared via solution casting method. The interactions between the polymer matrix and MgCl_2 salt was confirmed by Fourier Transform Infrared (FTIR) spectroscopy, while a mixed amorphous–crystalline structure, indicating effective ionic movement by X-ray Diffraction (XRD) analysis. Thermal stability of the pure PG film withstands till 250 °C by using Thermogravimetric Analysis (TGA). The correlation between the ionic movement and the surface morphology was explained by 3D Laser profilometry. A maximum ionic conductivity of $1.79 \times 10^{-3} \text{ S cm}^{-1}$ for the optimized configuration (PGMCSN5) was recorded by Electrochemical impedance spectroscopy (EIS). Dielectric properties, such as dielectric constant (ϵ_r) and dielectric loss (ϵ_i), were also evaluated via EIS data. The film exhibited a high ion transport number (TN) of 0.998, underscoring its efficiency in ion conduction. Overall, these results highlight PG-based biopolymer electrolytes as promising sustainable alternatives to conventional energy storage materials.

Keywords: Biopolymer electrolytes, Succinonitrile, Impedance studies, Magnesium salt, Transport number

| OP-25 |

E-Waste as a Circular Resource: Sustainable Metal Recovery Technologies and Material-Centric Challenges for Circular Economy Applications

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Abstract

Electronic waste is growing rapidly and has become a serious environmental challenge worldwide, while also representing an important secondary resource within circular economy frameworks. In recent years, extensive research has focused on recovering valuable metals from e-waste using sustainable, materials-chemistry-based approaches. Electronic waste is rich in valuable metals like copper, nickel, cobalt, iron, and precious metals, sometimes in higher concentrations than primary ores. This review examines global trends in e-waste generation alongside recent advances in sustainable metal recovery technologies, emphasizing materials chemistry. Environmentally benign recovery approaches, including advanced mechanical separation, hydrometallurgical, electrochemical, bio-leaching, and low-temperature processes, are critically discussed in terms of metal selectivity, recovery efficiency, energy demand, and environmental impact. The conversion of recovered metals into value-added materials, functional catalysts, and advanced material components for environmental remediation and energy applications is highlighted as a key pathway toward circular resource utilization. Despite substantial progress at laboratory and pilot scales, significant challenges persist related to feedstock heterogeneity, process scalability, economic feasibility, and integration with existing recycling infrastructures. Policy frameworks and extended producer responsibility initiatives are briefly discussed in relation to their role in supporting sustainable technologies. This review highlights key research gaps and future directions needed to convert e-waste from an environmental burden into a reliable and sustainable secondary resource. Emphasis is placed on materials chemistry perspectives that link recovery pathways with functional performance, environmental compatibility, and longterm resource efficiency across remediation, catalysis, and energy related material applications under realistic operational and sustainability constraints globally.

Keywords: Electronic waste, Sustainable, Circular economy, Environmental remediation

| OP-26 |

Fabrication of Novel Bi₂MoO₆/Nb₂CT_x Schottky Heterojunction Photocatalyst Toward Efficient Antibiotic Degradation

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Abstract

Heterojunction photocatalysts are promising materials for the degradation of detrimental antibiotic pollutants. In this study, a Bi₂MoO₆/Nb₂CT_x (BMO/NbC) Schottky heterojunction photocatalyst is reported for ciprofloxacin (CIP) and tetracycline (TC) degradation. Nb₂CT_x nanosheets were synthesized via HF etching, and layer-structured Bi₂MoO₆ nanosheets were in situ grown on different amounts of Nb₂CT_x nanosheets using a one-pot hydrothermal route to produce BMO/NbC hybrids. A large surface area with more active sites and extended visible light absorption was achieved by the 2D/2D (sheet-on-sheet) structure. Also, the Schottky barrier formed at the junction afforded a one-sided pathway for electron migration, thus preventing electron-hole recombination. Consequently, the BMO/NbC-50 hybrid (with 50 mg of Nb₂CT_x) unveiled excellent photocatalytic activity, achieving degradation removal efficiencies of 96.9% and 94.7% for CIP and TC, respectively, within 120 min. Moreover, the heterojunction photocatalyst exhibited good structural and chemical stability for up to five cycles. The photocatalytic mechanism was unlocked through band structure analysis. Scavenger test results revealed the participation of •O₂⁻, •OH, and h⁺ radicals in the degradation reaction. The fabricated Schottky heterojunction provides a potential contribution to environmental remediation through efficient antibiotic pollutant removal.

Keywords: Antibiotic; MXene; Photocatalytic degradation; Schottky heterojunction; Bi₂MoO₆

| OP-27 |

An Ultrasensitive Chromone-Derived Fluorescent Chemosensor for Cu²⁺ Detection Through LMCT: Real-World Applications and Computational Insights

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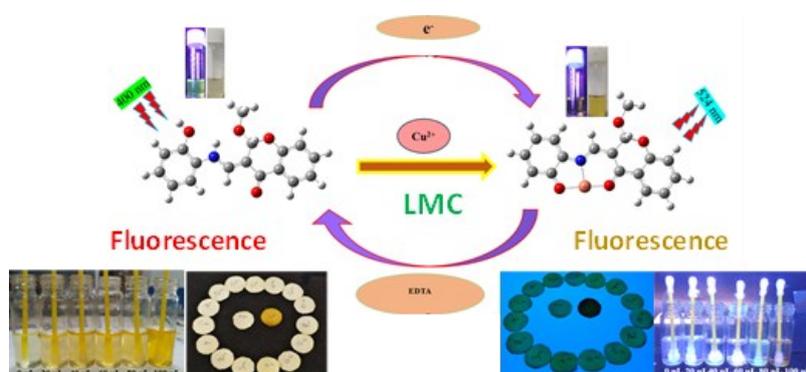
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Abstract

The pursuit of efficient molecular probes for transition metal ion detection is vital for environmental and biological safety. A novel chromone-derived Z-enamine probe, (Z)-3-(((2-hydroxyphenyl)amino)methylene)-2-methoxychroman-4-one (FCAP), was synthesized and structurally validated using FT-IR, NMR, LC-MS, and DFT studies. FCAP exhibits highly selective dual-mode sensing of Cu²⁺ ions, producing distinct colorimetric and fluorometric responses with negligible interference from other metal ions. Binding studies confirmed the formation of a strong 1:1 Cu²⁺-FCAP complex with a high binding constant ($K_a = 3.83 \times 10^7 \text{ M}^{-1}$) and an ultralow detection limit ($\text{LOD} = 1.97 \times 10^{-11} \text{ M}$). Mechanistic investigations revealed static fluorescence quenching via ligand-to-metal charge transfer. The probe demonstrates rapid response, excellent EDTA reversibility, and strong stability. Density functional theory (DFT) calculations further confirmed the enamine state of the molecule, supported by TD-DFT evidence and theoretical IR. Practical applicability was demonstrated through paper strip assays, smartphone-assisted detection, and real water sample analysis. Collectively, these findings establish FCAP as a promising, portable, and cost-effective sensing platform for reliable Cu²⁺ monitoring in environmental waters.

Keywords: Colorimetry, 2-Methoxy-3-enamine, Smartphone-based application, Theoretical calculation



| OP-28 |

Salt-Dependent Ionic Transport in Sodium Alginate Polymer Electrolytes: A Comparative Study of Sodium Bromide and Sodium Nitrite for Sodium-Ion Batteries

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Abstract

In response to increasing sustainability concerns, there is a growing shift from synthetic polymer-based electrolytes toward environmentally benign biopolymer electrolytes. Efficient ionic charge carriers are essential for enhancing ionic transport within polymer electrolyte systems. In this study, the influence of sodium bromide (NaBr) and sodium nitrite (NaNO₂) on the electrochemical performance of a sodium alginate polymer matrix was systematically investigated in the presence of a plasticizer. Sodium alginate–sodium bromide (SAB) electrolytes were initially prepared using a simple solution casting technique, followed by the fabrication of sodium alginate–sodium nitrite–ethylene carbonate (SANE) electrolyte systems. The prepared electrolytes were characterized using Fourier Transform Infrared Spectroscopy (FT-IR), Thermogravimetric Analysis (TGA), and 3D Optical Profilometry to evaluate their structural, thermal, and morphological properties. These analyses confirmed effective complexation between the ionic dopants and the host polymer matrix. Electrochemical performance was assessed through AC impedance spectroscopy, chronoamperometry, and linear sweep voltammetry to determine ionic conductivity, ionic transport number, and electrochemical stability window, respectively. Among the studied compositions, SAB-3 (60 wt% sodium alginate: 40 wt% NaBr) exhibited the highest ionic conductivity of $1.8 \times 10^{-3} \text{ S cm}^{-1}$ and a transport number of 0.81, surpassing SANE-3 (50 wt% sodium alginate: 45 wt% NaNO₂: 5 wt% ethylene carbonate), which showed $3.1 \times 10^{-4} \text{ S cm}^{-1}$ and 0.75, respectively. Primary sodium-ion batteries fabricated with Na|SAB-3|V₂O₅+graphite and Na|SANE-3|V₂O₅+graphite configurations delivered open-circuit voltages of 2.41 V and 2.32 V, with stability durations of approximately 152 h and 128 h, respectively, demonstrating the superior performance of the NaBr-based electrolyte system.

Keywords: Sodium alginate, Sodium bromide, Sodium nitrite, Ionic conductivity, Sodium-ion battery

| OP-29 |

Interfacial Charge Transfer and Oxygen-Vacancy Effects in Pd-Engineered ZnO during Ciprofloxacin Photodegradation

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Abstract

The present study reports the successful synthesis and comprehensive characterization of palladium-engineered zinc oxide nanostructures prepared via a simple oxalate precipitation method, with a focus on enhancing photocatalytic activity through improved charge separation. Structural analysis using X-ray diffraction confirmed the retention of the hexagonal wurtzite phase of Zinc Oxide after Pd incorporation, accompanied by slight lattice distortion and crystallite size reduction, indicating successful substitution and surface interaction of Pd within the ZnO matrix. FTIR identified the characteristic Zn–O stretching vibrations along with minor shifts caused by Pd modification. X-ray photoelectron spectroscopy (XPS) revealed the oxidation states of Zn²⁺, O²⁻, and Pd²⁺ and confirmed the formation of surface oxygen vacancies, which promote charge carrier transfer and improve photocatalytic activity. UV–Vis diffuse reflectance analysis confirmed the visible-light absorption enhancement of Pd–ZnO, arising from Pd-induced electronic coupling and improved charge-transfer efficiency. Photocatalytic degradation of ciprofloxacin (CIP) under natural sunlight irradiation demonstrated that the 0.1 wt% Pd–ZnO catalyst achieved superior efficiency, degrading 94.3% within 50 minutes under sunlight. The enhanced photocatalytic performance was attributed to effective charge carrier separation, suppression of electron–hole recombination, and increased production of reactive oxygen species ($\bullet\text{OH}$, $\text{O}_2\bullet^-$, and h^+). Reusability studies indicated excellent stability and retained activity over four consecutive cycles. Overall, the optimized 0.1 wt% Pd–ZnO photocatalyst exhibited high photocatalytic efficiency and good structural stability, demonstrating its potential applicability in wastewater treatment and environmental remediation.

Keywords: Palladium-engineered ZnO, Photocatalysis, Ciprofloxacin degradation, Visible-light photocatalyst, Environmental remediation, Wastewater treatment

| OP-30 |

Membrane-Assisted Light-Adaptive Sm–ZnO Photocatalyst for Antibiotic and Dye Abatement Coupled with Efficient Pathogen Suppression

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Abstract

Persistent pharmaceutical residues like doxycycline antibiotics and recalcitrant organic dyes such as methylene blue have emerged as critical aquatic pollutants, raising global concerns owing to their resistance to conventional treatment processes and their profound ecological and health implications. Herein, pristine ZnO and samarium-modulated ZnO (Sm–ZnO) photocatalysts were successfully developed through a straightforward chemical synthesis and comprehensively characterized by XRD, FT-IR, Raman spectroscopy, FE-SEM, HR-TEM, EDS, XPS, UV–Vis diffuse reflectance, and photoluminescence techniques. The Sm–ZnO catalysts demonstrated exceptional photocatalytic capability, delivering $\approx 98\%$ degradation of doxycycline (40 ppm) under UV-C illumination within 120 min and near-quantitative removal of methylene blue (10 ppm) under solar irradiation in only 50 min, employing 30 mg catalyst in 100 mL solution at pH 5. The markedly enhanced performance of Sm–ZnO is ascribed to synergistic effects arising from band-structure modulation, efficient suppression of charge-carrier recombination, broadened optical absorption, and the creation of highly reactive surface sites. Reactive species trapping experiments and GC–MS analyses confirmed that superoxide ($O_2^{\bullet-}$) and hydroxyl ($\bullet OH$) radicals are the primary contributors to pollutant mineralization. The Sm–ZnO photocatalyst was further evaluated for membrane-assisted degradation. Beyond photocatalytic remediation, Sm–ZnO exhibited strong antibacterial efficacy against both Gram-positive and Gram-negative microorganisms, while maintaining excellent durability and catalytic consistency across repeated reuse cycles. Overall, this study positions Sm–ZnO as a versatile and high-performance photocatalyst for integrated antibiotic degradation, dye detoxification, and microbial inactivation, offering a promising pathway toward sustainable and advanced wastewater remediation technologies.

Keywords: Sm–ZnO photocatalyst, Membrane-assisted degradation, Doxycycline removal, Solar/UV-C photocatalysis, Antibacterial activity

| OP-31 |

Antimicrobial Characteristics of Molecular Complexes of Zn(II) And Cd(II) Metal Ions

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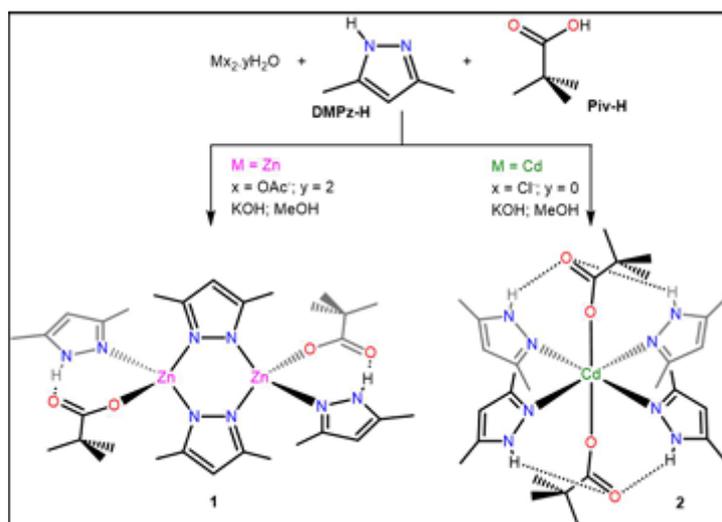
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Abstract

Here, we are presenting the synthesis, characterization, and evaluation of the antimicrobial and photophysical properties of Zn(II) and Cd(II) complexes (1 and 2 respectively) utilizing 3,5 dimethyl pyrazolate (DMPz-) and pivalate (Piv-) ligands. The complexes were synthesized through a straightforward coordination reaction by a one pot mixing of metal salt and ligands at room temperature. Their structural integrity was confirmed using spectroscopic techniques, including, IR, UV-Visible, Fluorescence, and NMR spectroscopy as well as single-crystal X-ray diffraction analysis. The antimicrobial activity of the synthesized complexes was evaluated against a range of bacterial and fungal strains using standard antimicrobial assays. The results revealed significant antimicrobial efficacy for both complexes 1 and 2, with variations in effectiveness depending on the metal center and the coordination behaviour of the ligands in the solution.

Keywords: Sm–ZnO photocatalyst, Membrane-assisted degradation, Doxycycline removal, Solar/UV-C photocatalysis, Antibacterial activity



| OP-32 |

Environmental Remediation of Heavy Metals from Effluents Through Metal Organic Frameworks

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Abstract

Heavy metal contamination is a major global environmental challenge that affects ecosystems and disrupts the cellular homeostasis of living organisms. Metal-organic frameworks with their high porosity, large surface area, and tunable pore structures offer an excellent platform that effectively address on heavy metal remediation. MOFs were prepared with dicarboxylate organic linker such as 9,10-Anthracene dicarboxylic acid and with metal nodes [M=Europium and Terbium]. The formation of these complexes has been confirmed using various spectral techniques. FTIR for all the complexes observed transmittance in the range 1408-1590 cm^{-1} were corresponding to symmetric and asymmetric stretching frequency of carboxylate group and 430 -481 cm^{-1} were confirming the metal oxygen bond. PXRD pattern showed diffraction peaks which confirms high crystallinity and phase purity with corresponding miller indices values like [331, 110, 310, 210]. UV-Visible spectroscopy of all complexes showed intense excitation wavelength range between 223 to 225nm was due to π - π^* and n - π^* transition of the ligand and its binding towards the metal nodes. And the corresponding emission wavelength was found to be at 420nm. The results exhibits that prepared MOF involve ligand-to-metal charge transfer were d orbitals of metals interact with inner f orbitals of organic linker via antenna effect. Morphological studies reveal angular crystalline polyhedral faceted surface with an elongated platelet with well-defined crystal faces. Fluorescence studies were carried out to detect the heavy metals present in industrial effluents which contain Zn, Ni, Cr metals through regular intervals of time (2h, 4h, 6h and 24 h). After 24 hours of adsorption, the intensity showed removal efficiencies of Zn 59.44%, for Ni metal 98.38% and 98.55% for chromium. Among the four MOF's Eu-ADC MOF exhibited superior adsorption performance toward Cr metal, whereas Tb-ADC MOF showed excellent adsorption efficiency for Ni metal. The adsorption efficiency may be due to pores of the MOF allowed to trap contaminants like a sponge enter and interact, luminescent properties get disturbed and leading to photoluminescence quenching.

Keywords: Metal organic frameworks, Environment impacts, Effluents, Public health, Risk assessment

| OP-33 |

Rational Design of MoWS₂/NiMoO₄ Hybrid Electrodes with Enhanced Interfacial Coupling for Energy Storage Applications

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Abstract

The development of high-performance electrode materials is crucial for next-generation energy storage systems. In this study, a novel two-dimensional (2D) MoWS₂/NiMoO₄ nanocomposite was synthesized and evaluated for supercapacitor applications. The hybrid structure combines the excellent electrical conductivity and large surface area of layered MoWS₂ with the rich redox activity and high theoretical capacitance of NiMoO₄. The nanocomposite was prepared via a facile two-step hydrothermal method and achieved strong interfacial coupling between the components. Structural and morphological analyses confirmed the successful formation of a cubic structure on nanorods with a sheet-like architecture, facilitating efficient ion diffusion and rapid charge transport. Electrochemical measurements revealed a high specific capacitance of 2974 F g⁻¹ at 1 A g⁻¹ and maintained 85.5% capacity retention after 5000 cycles at 10 A g⁻¹ in 6 M KOH. The synergistic interaction between MoWS₂ and NiMoO₄ enhances electron transport pathways and provides multiple Faradaic redox reactions, leading to superior energy storage performance. The assembled device demonstrated high energy density and excellent long-term stability, indicating the promising potential of 2D MoWS₂/NiMoO₄ nanocomposites as advanced electrode materials for high-performance supercapacitors.

Keywords: MoWS₂, Supercapacitor, Nanocomposites

| OP-34 |

Development of Value-Added Carbon Dots from Renewable Plant Waste at PSGCAS through Green Method for Real Time Bioimaging Applications

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Abstract

Luminescent carbon dots (C-dots) are emerging as versatile nanomaterials for bioimaging, sensing and biomedical applications due to their excellent photoluminescence, water solubility, biocompatibility, low toxicity and cost-effectiveness. In this study, value-added fluorescent carbon dots were developed through a green, hydrothermal synthesis using renewable plant waste generated within the PSGCAS campus, thereby converting local biomass waste into a high-value nanomaterial with minimal environmental impact. The synthesized C-dots were then characterized using UV-visible spectroscopy, photoluminescence spectroscopy, scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), and transmission electron microscopy (TEM) to confirm their optical properties, morphology, and elemental composition. The synthesised C-dots exhibited strong fluorescence under UV light, nanoscale dimensions and good aqueous dispersibility, indicating successful synthesis and stability. Furthermore, the MTT cytotoxicity assay showed no significant reduction in cell viability, confirming that the synthesized C-dots are non-toxic at the tested concentrations. The work highlights a sustainable strategy for recycling institutional plant waste into functional nanomaterials and addresses a critical research gap by focusing on waste-derived C-dots for biomedical imaging. This approach aligns with the UN Sustainable Development Goals (SDGs 3, 9, 12, 13 and 15) by promoting green nanotechnology, sustainable waste utilization and eco-friendly healthcare solutions.

Keywords: Carbon dots, MTT assay, Biomedical applications

| OP-35 |

Bio-Derived Trifunctional Sustainable Benzoxazines for Corrosion Protection and Multifunctional Surface Applications

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Abstract

Sustainable coating materials that combine durability, functionality and reduced processing demands are receiving increasing attention for protective applications. In this work, a tri functional phenol precursor was synthesized from 2-allyl phenol and bio-derived 3-ethyl vanillin and subsequently converted into three benzoxazine systems using furfurylamine, 3-aminothiophenol, and aniline. The resulting polybenzoxazines were studied to understand how amine structure influences curing behaviour, surface properties, and long-term coating performance. The furfurylamine-based benzoxazine exhibited the lowest curing temperature of 223°C suggesting reduced energy requirements during coating fabrication. In contrast, the aniline-derived system showed superior thermal stability, delivering a char yield of 43% and a maximum degradation temperature of 470°C, which is favorable for extended service life under demanding conditions. All coatings displayed pronounced water repellence, with water contact angles exceeding 140°, indicating the formation of compact and chemically robust surfaces. From an application standpoint, fabrics coated with the 3-aminothiophenol-based polybenzoxazine achieved an oil-water separation efficiency of 96%. In addition, all of the polybenzoxazine coatings provided excellent corrosion protection on mild steel with inhibition efficiencies of up to 99% and also exhibited effective antibacterial activity. Overall, the incorporation of a bio-based trisphenol structure combined with tunable amine chemistry enables the development of multifunctional polybenzoxazine coatings that support sustainable processing, enhanced durability and reduced material usage in protective and separation related applications.

Keywords: Sustainable polybenzoxazines, Hydrophobicity, Oil water separation, Anticorrosion, Antibacterial activity

| OP-36 |

Synthesizing a Luminescent Copper Metal-Organic Framework and Utilizing It for the Fluorescent Detection and Discrimination of Ethanol and Methanol

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Abstract

Luminescent metal-organic frameworks (MOFs) are promising materials for fluorescence-based chemical sensing because of their structural tunability and strong emission properties. In this study, a copper-based luminescent MOF (Cu-MOF) was synthesized using a simple interfacial layering technique with copper iodide and 4-picolyamine. The synthesized framework formed a two-dimensional coordination network and exhibited good thermal stability along with intense green fluorescence in the solid state. The fluorescence sensing behavior of the Cu-MOF was explored for methanol and ethanol, which are significant volatile organic compounds in environmental and forensic contexts. The variation in fluorescence response enabled clear discrimination between methanol and ethanol, indicating the selective recognition capability of the framework toward closely related alcohols. The developed Cu-MOF demonstrates several advantages such as rapid response, strong emission intensity, and good stability. These features make it potential for use as a fluorescent probe for the detection and differentiation of toxic alcohols. This work highlights a straightforward approach for the development of luminescent MOF-based sensing materials for selective volatile organic compound detection. The results presented here may support future applications in environmental monitoring, industrial safety, and forensic analysis, and contribute to the ongoing design of functional luminescent coordination frameworks for practical sensing platforms.

Keywords: Metal organic framework, Photoluminescence, Copper iodide, Picolyamine

| OP-37 |

Electrolyte-Driven Modulation of Redox Kinetics Governing Charge Storage in Copper Manganese-based Prussian Blue Analogues for Aqueous Potassium-Ion Batteries

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Abstract

Prussian blue (PB) and its analogues have emerged as promising electrode materials for metal ion batteries due to their facile synthesis, abundant redox-active sites, and structural robustness during repeated cycling. Despite this, strategies to enhance their electrochemical performance via electrolyte engineering remain limited. Herein, we report the synthesis of potassium copper manganese hexacyanoferrate (KCuMnHCF, denoted as KCM), a PB-based compound, via a straightforward co precipitation route, and its evaluation as a cathode material for aqueous potassium-ion energy storage. Comprehensive physicochemical characterizations were performed to elucidate the crystal structure, morphology, and surface characteristics of KCM. The electrochemical performance was systematically assessed in aqueous KOH electrolyte and in KOH containing redox-active additives, specifically potassium ferrocyanide ($K_4[Fe(CN)_6]$) and potassium ferricyanide ($K_3[Fe(CN)_6]$). Cyclic voltammetry and galvanostatic charge–discharge measurements revealed that electrolyte composition plays a critical role in modulating charge-storage behavior. Comparative analysis identified the most effective electrolyte system for enhanced capacity and cycling stability. These findings highlight the synergistic potential of PB-based cathodes and tailored electrolyte design, providing a promising pathway toward high-performance aqueous potassium-ion energy-storage systems.

Keywords: Prussian blue analogue, Aqueous K-ion batteries, Redox kinetics, Energy storage.

| OP-38 |

Dielectric and conductivity studies of *Pterocarpus marsupium* gum doped with NaClO₄

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Abstract

Solid biopolymer electrolytes have gained much attention in recent years. Due to their various advantages, they can be used in advanced electrochemical devices. The present study focuses on the conductivity and dielectric properties of *Pterocarpus marsupium* gum doped with NaClO₄. Different concentrations of sodium perchlorate (NaClO₄) were added to the PVA+*Pterocarpus marsupium* gum solution and stirred until complete dissolution. The homogeneous solutions were then placed onto different plastic Petri dishes, where they were left to dry. The highest biopolymer electrolyte possesses an optimum ionic conductivity value of the order of $2.56 \times 10^{-6} \text{ S cm}^{-1}$ as observed by the AC impedance spectroscopy analysis at room temperature. Dielectric and conductivity studies were also performed in the frequency range of 300 Hz - 4 MHz.

Keywords: Biopolymers, AC impedance analysis, Conductivity, Dielectric studies.

**POSTER
PRESENTATIONS**

| PP-01 |

Green-Synthesized B/N co-Doped Carbon Quantum Dots for Dual Fluorescence Sensing of Phenothiazine Drugs and Hg²⁺ Ions

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Abstract

Pharmaceutical pollutants and Hg²⁺ ions are persistent environmental contaminants requiring rapid, sensitive, and selective detection. This study presents a green one-pot hydrothermal synthesis of B/N co-doped carbon quantum dots (B/N-CQDs) using biomass-derived, non-toxic precursors, avoiding hazardous reagents and post-modification steps. The dots display strong blue photoluminescence (~440 nm at 360 nm excitation), quantum yield ~20%, high water dispersibility, photo-stability, and salt tolerance, attributed to efficient heteroatom doping and abundant surface groups (-OH, -COOH, -NH₂, B-induced Lewis acid sites). Phenothiazine drugs (promethazine, chlorpromazine) are detected through Inner Filter Effect (IFE)-driven fluorescence modulation due to absorption overlap at 250–350 nm, producing a linear range of 0.05–25 μM with LOD ~25 nM. Hg²⁺ sensing occurs via static quenching through strong coordination with N/B-rich sites forming non-emissive ground-state complexes, giving a linear range of 0.01–10 μM and LOD ~5 nM. The probe delivers ultrafast response (<30 s), excellent selectivity, and reversible recovery using EDTA chelation. Validation in spiked tap/lake water and serum matrices shows 95–103% recovery, confirming accuracy and matrix compatibility. The B/N-CQD sensor offers a low-cost, non-toxic, and scalable fluorescence platform for dual environmental surveillance and bioanalytical monitoring of phenothiazine residues and mercury contamination.

Keywords: B/N co-doped carbon quantum dots, Green hydrothermal synthesis, Inner Filter Effect (IFE), Phenothiazine drug sensing, Mercury ion detection (Hg²⁺).

| PP-02 |

CeO₂ Nanoparticles Decorated on CoAl-LDH Hexagonal Nanosheets as a High-Performance Hybrid Electrode for Supercapacitors

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Abstract

A rationally integrated 0D/2D hierarchical composite electrode was developed by uniformly decorating CeO₂ nanoparticles (5–8 nm, fluorite phase) onto CoAl - Layered Double Hydroxide (CoAl-LDH) hexagonal nanosheets (120–180 nm lateral size, 8-12 nm thickness, BET surface area 142 m² g⁻¹) via a solvothermal deposition process (160°C, 12 h). Structural and defect analysis by XPS confirms Ce⁴⁺/Ce³⁺ coexistence with abundant oxygen-vacancy (O_v) sites (Ce³⁺ fraction: 28.4%), while Raman spectroscopy evidences F_{2g} lattice vibration at 462 cm⁻¹, validating strong interfacial coupling and defect-assisted conductivity. The composite exhibits enhanced electrical conductivity (1.8 × 10⁻² S cm⁻¹) compared to pristine LDH (4.6 × 10⁻³ S cm⁻¹). In 3M KOH aqueous electrolyte, the CeO₂/CoAl-LDH electrode delivers a high specific capacitance of 1,246 F g⁻¹ at 1 A g⁻¹, retaining 812 F g⁻¹ at 20 A g⁻¹ (65.2% retention), surpassing bare CoAl-LDH (732 F g⁻¹ at 1 A g⁻¹). Electrochemical impedance spectroscopy reveals low equivalent series resistance (ESR-0.42Ω) and reduced charge-transfer resistance (R_{CT}-0.87Ω), indicating accelerated ion/electron transport. A symmetric supercapacitor device assembled using the hybrid electrode achieves energy densities of 42.8 Wh kg⁻¹ at 750 W kg⁻¹ and 16.3 Wh kg⁻¹ at 15 kW kg⁻¹, with 93.6% capacitance retention over 10,000 GCD cycles at 10 A g⁻¹ and Coulombic efficiency > 98%. The performance enhancement is attributed to oxygen-vacancy-mediated conductivity of CeO, synergistic Co²⁺/Co³⁺ Faradaic redox activity, and short ion-diffusion pathways of the 2D LDH scaffold, demonstrating strong potential for durable, high-capacitance alkaline supercapacitor energy-storage applications.

Key Words: CeO₂ nanoparticles, CoAl-LDH nanosheets, 2D/0D hybrid electrode, Oxygen vacancies, Alkaline supercapacitor.

| PP-03 |

New Insights into Continuous Flow Reactor Systems for the Effective Degradation of Persistent Pharmaceutical Pollutants Using Advanced Oxidation Processes

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Abstract

The widespread use of antibiotics in human and veterinary medicine has led to their persistent release into the environment through wastewater and agricultural runoff. Antibiotics such as tetracycline (TC) have been detected in surface water, groundwater, and even drinking water due to their incomplete removal by conventional wastewater treatment processes. These challenges underscore the need for innovative and efficient treatment technologies to address the persistent environmental contamination caused by antibiotics. To resolve this issue, this study explores the combination of ultrasound with S-scheme $\text{CoFe}_2\text{O}_4(\text{CFO})/\text{Bi}_2\text{WO}_6(\text{BWO})$ heterostructures to effectively degrade refractory organic pollutants such as TC. The CFO in this system transfers electrons to BWO, facilitating efficient charge separation through an internal electric field. The integration of ultrasound with the CFO/BWO heterostructure significantly boosts the generation of reactive oxygen species, thereby improving the degradation of TC. Comprehensive characterization confirmed the catalyst's structural, optical, thermal and electrochemical properties. The operational parameters were optimized, and the catalyst demonstrated excellent stability and reusability over multiple cycles. Importantly, the toxicity studies were evaluated using zebrafish embryo studies, confirming the safety of treated water for environmental release. Additionally, the continuous flow sono-photocatalytic reactor successfully mineralized the pharmaceutical effluent. This approach presents a promising solution for TC degradation and other emerging contaminants.

Keywords: Ultrasound, Sono-photocatalysis, Continuous flow sono-photocatalytic reactor, Zebrafish, S-scheme heterojunction, Cobalt ferrite, Bismuth tungstate

| PP-04 |

Nitro quinolone Fused Salicyl and Naphthyl Hydrazone Fluorescent Probes for the Detection of Fe³⁺ and Pb²⁺ Ions

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Abstract

The application of quinolones stretches over a large umbrella of medicinal field as well as chemosensor due to the presence of privileged heterocyclic aromatic ring system. Salicyl and Naphthyl Hydrazone motifs are also established fluorophore groups. Therefore in this work, we have designed and synthesized Salicyl hydrazone (**3a-c**) and naphthyl hydrazone fused nitro quinolones (**5a-c**) investigated for their fluorescent behaviour. Preliminary absorption studies were carried out and the metal selectivity were examined with various metal ions. Among them, it was found that compound **3a** was selective towards Fe³⁺ ions ($\lambda_{ex} = 330$ nm, 1:1 DMF:H₂O at pH = 7.4 in HEPES Buffer medium) showing a quenching of emission intensity while compound **5a** was selective towards Pb²⁺ ion ($\lambda_{ex} = 280$ nm, 1:1 DMF:H₂O at pH = 7.4 in HEPES Buffer medium) showing an enhancement in fluorescence intensity. Further, the concentration dependence, competitive binding and EDTA reversibility were studied for selected compounds towards the respective cation's selectivity. Jobs plot analysis indicates that 1:1 binding of **3a** with Fe³⁺ ion ($K_a = 3.17 \times 10^4$ M⁻¹ and LOD = 5.1×10^{-7} M) whereas **5a** showed 1:2 binding mode with Pb²⁺ ions ($K_a = 2.14 \times 10^6$ M⁻¹ and LOD = 2.613×10^{-9} M). Density Functional Theoretical studies were performed as a theoretical support for the experimental results.

Keywords: Hydrazones, Lead, Iron, Fluorescence, Chemosensors, PET, DFT

| PP-05 |

Ligand-Engineered Homoleptic Co(III) Complexes Based on Salicylamine-Schiff Bases for Oxygen Evolution Electrocatalysis

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Abstract

The development of efficient and sustainable electrocatalyst for the Oxygen Evolution Reaction (OER) is essential for advancing renewable energy technologies. In this work, two homoleptic cobalt(III) complexes were synthesized using Schiff base ligands derived from flexible salicylamine derivatives and bulky 3,5-di-tert-butylsalicylaldehyde. Complex 1 originates from 3-methoxysalicylamine and 3,5-di-tert-butylsalicylaldehyde ($L^{\text{OMe}}\text{H}_2$), while complex 2 is based on 3-ethoxysalicylamine and the same aldehyde precursor ($L^{\text{OEt}}\text{H}_2$). This ligand design provides a balance between electronic stabilization and structural flexibility, enabling the formation of active catalytic sites under operational conditions. Single-crystal X-ray diffraction confirmed that both complexes adopt a distorted octahedral coordination geometry in the +3-oxidation state, with triethylammonium cations serving as charge-balancing counter ions. Electrochemical measurements revealed promising OER performance, with over-potentials of 334 mV and 348 mV at 10 mA cm^{-2} and Tafel slopes of 63 and 70 mV dec^{-1} for complexes 1 and 2, respectively. Turnover frequency analysis reveals higher intrinsic catalytic activity for complex 1. Post-catalytic SEM, XPS, and PXRD analyses indicate that both complexes preserve their structural integrity and coordination environments, demonstrating excellent stability under OER conditions. These results highlight the potential of cobalt-based molecular complexes as cost-effective and earth-abundant electrocatalysts for sustainable energy conversion.

Keywords: Homoleptic metal complexes, Molecular electrocatalyst, Water oxidation, Turnover frequency, Ligand engineering

| PP-06 |

Quinoline-Dipeptide Conjugated Scaffolds as Effective Uric Acid Sensors

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Abstract

Quinoline and peptide conjugated compounds represent an important class of hybrid molecules that combine the advantages properties of heterocyclic scaffolds with the high specificity and biocompatibility of peptides. Synthesis of quinoline starts with precursor 2-hydroxy, 4-mehtyl quinoline which was oxidized using KMnO₄ to yield 2- hydroxy quinoline -4- carboxylic acid which in turn converted to acid chloride. For peptide synthesis liquid phase synthesis was opted. Herein we conjugated the dipeptide with the quinoline carboxy chloride. The synthesised compounds were characterized by UV, IR, 1H & 13C NMR. The synthesised compounds were tested for their effectiveness to sense Uric acid by, UV detector, UV Visible, PL spectroscopy and Electrochemical technique. The details on synthesis, Characterization and sensor application are to be explained

Keywords: Quinoline, Dipeptide, Sensors.

| PP-07 |

Applications of Click Chemistry in Modern Drug Discovery and Targeted Drug Delivery: A Review

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Abstract

Click chemistry has become a transformative strategy in modern drug discovery and drug delivery due to its exceptional efficiency, selectivity, and compatibility with biological systems. Click reactions, which are characterized by their quick reaction rates, high yields, and few by-products, allow for the accurate formation of complex molecular structures under mild circumstances. Among these, azide–alkyne cycloaddition reactions both copper-catalysed and metal-free variants are extensively employed for the modular synthesis of drug candidates, prodrugs, and functional biomolecules. In drug discovery, click chemistry facilitates lead optimization, structure activity relationship studies, and the rapid generation of compound libraries with enhanced pharmacological properties. In drug delivery applications, it plays a crucial role in the construction of targeted delivery systems, including polymer drug conjugates, nanoparticles, antibody drug conjugates, and stimuli-responsive carriers, thereby improving therapeutic efficacy and reducing off-target toxicity. Furthermore, bio-orthogonal click reactions allow in situ conjugation and real-time tracking of drugs within living systems without disrupting native biochemical processes. This review highlights the growing significance of click chemistry as a versatile and powerful platform that bridges synthetic chemistry and biomedical innovation, offering promising solutions for the development of next-generation therapeutics.

Keywords: Click chemistry, Drug discovery, Drug delivery, Drug candidates

| PP-08 |

The Effect of the Unsaturated Polyester Resin in Carbon Doped MgO as a Electrocatalyst in the Aluminium Air Battery

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Abstract

Recently, aluminium- air batteries (AABs) have drawn a lot of attention due to their inexpensive cost and high energy density. For years, aluminium- air batteries have been at the forefront of energy research due to their high theoretical specific volumetric capacity, making them an interesting alternative to lithium-based energy storage. Because of its large volumetric and gravimetric capacity, aluminium is used as an anode material. Additionally, a solid state - aluminium air battery could prevent leaks, enhance safety and facilitate widespread use. Even more remarkable is the assembly of a sophisticated flexible aluminium-air battery with good cycling stability and a maximum power density. The essential components in Al air battery are the aluminium anode. The air cathode comprises of an oxygen reducing catalyst, a current collector and a composite electrode, like C/Mg (NO₃)₂ to use various carbon Like, KS44, N330, Super P carbon doped with metal oxide to bind with GPR resin. In use alkaline electrolyte such as potassium hydroxide (KOH) in Aluminium air battery has one of the highest energy density among battery technology making them suitable for application requiring long-lasting power. To use middle layer of the separator like AGM (Absorbent glass mat) is a type of nanofiber material to use to keep the two electrodes apart. The aluminium goes through an oxidation reaction the release electrode that moves through an external circuit to do work. The electrochemical stable window covers redox voltage of most reported cathode material like, unsaturated polyester polymer at aluminium air battery can be good candidate. Furthermore, in the Al air cell the longest discharge voltage time was unsaturated polyester polymer with C/Mg (NO₃)₂ and 1 M of KOH in which the cell voltage was maintained at 1.81V to 1.53 V for almost 168 hours.

Keywords: Polyester Resin, Carbon KS44, Carbon N330, Magnesium Oxide, Al-air battery

| PP-09 |

Environmental Forensic Investigation of Toxic Plastic Ingestion in Wildlife Using Spectral and Thermal Analysis

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Abstract

The occurrence of anthropogenic plastic residues within forest ecosystems is an increasing environmental and toxicological concern, particularly when such materials interact with wildlife. The present investigation focuses on the chemical and thermal characterization of a plastic residue isolated from elephant (*Elephas maximus*) dung collected from a forested region, using Fourier Transform Infrared Spectroscopy (FTIR) and Thermogravimetric Analysis (TGA). FTIR spectral analysis of the recovered material revealed prominent absorption bands characteristic of long-chain aliphatic polymers. Strong C–H stretching vibrations were observed in the region of 2915–2848 cm⁻¹, accompanied by deformation bands near 1470 cm⁻¹ and a distinct absorption around 720 cm⁻¹ corresponding to $-(CH_2)-$ rocking vibrations. The lack of significant absorptions related to polar functional groups suggests a chemically inert, non-polar polymeric material with limited oxidative modification. These features are indicative of a polyolefin-based plastic, showing close similarity to polyethylene-type polymers. Thermogravimetric analysis demonstrated a single-step thermal degradation pattern, with minimal weight loss at lower temperatures and rapid decomposition occurring at higher temperatures. This degradation behavior reflects high thermal stability, consistent with polyethylene-dominant plastic materials, particularly those resembling high-density polyethylene (HDPE). The integrated spectroscopic and thermal findings confirm the persistent and synthetic nature of the plastic residue ingested by wildlife, emphasizing its resistance to environmental degradation within forest ecosystems. This study highlights the effectiveness of FTIR and TGA as complementary analytical tools for identifying plastic contamination in wildlife-associated samples and reinforces the importance of monitoring anthropogenic pollutants in ecologically sensitive habitats.

Keywords: Wildlife exposure, Forest ecosystem, Plastic residues, FTIR, Thermogravimetric analysis, Environmental toxicology

| PP-10 |

In-Vitro Studies of PVA-Chitosan Nanofibers Infused with *Neem* and *Aloe vera* for Advanced Antimicrobial Protection

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Abstract

Polyvinyl alcohol (P)/Chitosan (C) electrospun nanofibers, composed of neem (N) extract and aloe vera (A) gel, represent a promising biocompatible platform for antimicrobial wound dressings and other biomedical applications. In this study, six nanofiber mat formulations (PA, PC, PN, PCN, PCA, and PCAN) were prepared by electrospinning by varying the concentrations of chitosan, neem extract, and aloe vera extract while maintaining a constant polyvinyl alcohol content, with optimized polymer blend compositions to enhance bioactivity, mechanical integrity, and thermal stability. The fabricated nanofibrous mats exhibited excellent antimicrobial performance. Antibacterial activity against *Klebsiella pneumonia* and *Escherichia coli*, as well as antifungal activity against *Candida albicans*, was analyzed. Cytotoxicity assessment using the MTT assay confirmed the high cell viability, indicating good biocompatibility of the developed fabrics. The morphology, thermal performance, and bonding interactions of the fabricated sample were thoroughly evaluated. Scanning electron microscope (SEM) images revealed the formation of uniform bead-free nanofibers with an average diameter of approximately 131nm, ranging from 100 nm to 190 nm. Fourier Transform Infra-Red (FTIR) Spectroscopy confirmed the successful incorporation of neem polyphenols and aloe vera polysaccharides into the CS matrix, evidenced by characteristic O-H and N-H stretching vibrations around 3400 cm⁻¹. Tensile testing further demonstrated enhanced superior mechanical properties. Overall, the results indicate that fabricated electro spun scaffolds possess significant potential for wound dressing applications, offering antimicrobial efficiency, biocompatibility, and structural integrity, thereby supporting their suitability for scalable biomedical translation.

Keywords: Electrospun nanofiber, Antibacterial, Antifungal, Biomedical, Cytotoxicity

| PP-11 |

Tungsten-Cobalt Oxalate with Multiple Catalytic Sites as Efficient Electrocatalyst for Boosting Overall Water Splitting

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Abstract

Pharmaceutical pollutants and Hg²⁺ ions are persistent environmental contaminants requiring rapid, sensitive, and selective detection. This study presents a green one-pot hydrothermal synthesis of B/N co-doped carbon quantum dots (B/N-CQDs) using biomass-derived, non-toxic precursors, avoiding hazardous reagents and post-modification steps. The dots display strong blue photoluminescence (~440 nm at 360 nm excitation), quantum yield ~20%, high water dispersibility, photostability, and salt tolerance, attributed to efficient heteroatom doping and abundant surface groups (–OH, –COOH, –NH₂, B-induced Lewis acid sites). Phenothiazine drugs (promethazine, chlorpromazine) are detected through Inner Filter Effect (IFE)-driven fluorescence modulation due to absorption overlap at 250–350 nm, producing a linear range of 0.05–25 μM with LOD ~25 nM. Hg²⁺ sensing occurs via static quenching through strong coordination with N/B-rich sites forming non-emissive ground-state complexes, giving a linear range of 0.01–10 μM and LOD ~5 nM. The probe delivers ultrafast response (<30 s), excellent selectivity, and reversible recovery using EDTA chelation. Validation in spiked tap/lake water and serum matrices shows 95–103% recovery, confirming accuracy and matrix compatibility. The B/N-CQD sensor offers a low-cost, non-toxic, and scalable fluorescence platform for dual environmental surveillance and bioanalytical monitoring of phenothiazine residues and mercury contamination.

Keywords: B/N co-doped carbon quantum dots, Green hydrothermal synthesis, Inner Filter Effect (IFE), Phenothiazine drug sensing, Mercury ion detection (Hg²⁺).

| PP-12 |

Synergistic Integration of $\text{LaMnO}_3@ \text{NiCo}_2\text{O}_4$ Heterostructures with rGO for Efficient Hybrid Supercapacitors

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Abstract

Electrochemical energy storage systems (EESSs) play a critical role in addressing environmental issues by enabling the efficient use of renewable energy sources and reducing reliance on fossil fuels. Depending on the design and functioning, these systems can provide high energy density or high-power density, like batteries and supercapacitors. Copious materials and media have been tested and trialled. Transition metal oxides (TMOs) such as perovskites, spinels, etc have been explored extensively as electrode materials for supercapacitors due to their rich redox chemistry. Prominent metals such as Mn, Ni, Co, and Fe are often employed as a positive electrode, whereas carbonaceous materials such as graphene, rGO, and others are used on the negative electrode of the electrochemical system. The overall electrochemical property is improved by combining various components to form a novel substance recognised as a heterostructure composite. Herein, the integration of LaMnO_3 based perovskite and NiCo_2O_4 -based spinel, along with the rGO, into a composite via a facile hydrothermal method. Several structural characterisations are used to have an extensive comprehension of the material. The electrochemical study is carried out in an aqueous medium, using both three and two-electrode systems. The specific capacitance of the composite is 600 F g^{-1} at 1 A g^{-1} in the 0.4 V to -0.5 V potential window. The capacitance retention is nearly 96% achieved at 2000 cycle stability test. The maximum energy density is 254 Wh kg^{-1} , with a power density of $1.9 \times 10^4 \text{ W kg}^{-1}$. Such ubiquitous electrochemistry will potentially play an important role in generating sustainable energy storage systems in the near future.

Keywords: Perovskite, Spinel, Heterostructures, Hybrid Supercapacitors and Asymmetric electrode system.

| PP-13 |

Green Conversion of Carbon Dioxide to Formic Acid via Metal Complex Catalyzed Hydrogenation

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Abstract

The sustainable conversion of carbon dioxide into value-added chemicals is a key challenge in carbon capture and utilization strategies. Formic acid is an attractive product owing to its high volumetric hydrogen density, low toxicity, and direct applicability in hydrogen storage and fuel cell technologies. In the present work, an efficient and sustainable catalytic system for the hydrogenation of carbon dioxide to formic acid using a transition-metal coordination complex is reported. The metal complex catalyst enables CO₂ activation and hydrogenation under relatively mild conditions (60–80°C and 30–50 bar total pressure), achieving a formic acid yield of 96% with selectivity exceeding 99%. A maximum turnover number (TON) of 15,200 and a turnover frequency (TOF) of 2,850 h⁻¹ were obtained, indicating high catalytic efficiency and stability. Compared with conventional heterogeneous catalysts such as supported noble metals (Pd/C, Ru/C), which typically require higher temperatures (140 °C) and pressures (>80 bar) with moderate selectivity, the present metal complex system operates under significantly milder conditions while delivering superior selectivity toward formic acid. In contrast to enzymatic and electrochemical CO₂ reduction routes that suffer from low current efficiency or complex reactor design, the proposed catalytic process offers a simple reaction setup, high atom economy, and excellent catalyst recyclability, retaining over 90% of its activity after five successive cycles. Mechanistic studies suggest a metal–hydride mediated pathway involving CO₂ insertion into a metal–hydride intermediate followed by protonation, enabling efficient catalyst regeneration. This work demonstrates a viable, low-energy, and environmentally benign route for formic acid production from CO₂ and hydrogen, highlighting the potential of metal complex catalysts for scalable carbon-neutral chemical and energy applications.

Keywords: Metal hydride, CO₂ activation, Energy applications

| PP-14 |

Metal Carbamate Complexes as Cholinesterase Inhibitors: An ANN-Based Predictive Study

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Abstract

Metal carbamate complexes have emerged as promising candidates for cholinesterase inhibition due to their tunable coordination environments and enhanced interaction with enzyme active sites. In the present study, a series of metal–carbamate complexes were synthesized and evaluated for their inhibitory activity against acetylcholinesterase (AChE) and butyrylcholinesterase (BChE). The inhibitory efficiency was experimentally determined using Ellman’s spectrophotometric assay, and the resulting IC₅₀ values were employed to develop an Artificial Neural Network (ANN)–based predictive model. Physicochemical and structural descriptors, including metal ion properties, ligand parameters, coordination geometry, molecular weight, and experimental conditions, were used as input variables. A multilayer feed-forward ANN with a single hidden layer was trained using the Levenberg–Marquardt and Scaled Conjugate Gradient algorithms, yielding excellent correlation between predicted and experimental inhibition data. The optimized model exhibited high regression coefficients and low mean squared error, demonstrating strong predictive capability. Sensitivity analysis revealed that metal ion characteristics and ligand electronic properties play a dominant role in cholinesterase inhibition. The ANN model effectively reduced experimental trial-and-error and enabled rapid screening of potent metal–carbamate inhibitors. This integrated experimental and computational approach provides valuable insights into structure–activity relationships and offers a cost-effective strategy for the rational design of metal-based cholinesterase inhibitors for neurodegenerative disease management.

Keywords: ANN, Metal carbamate, Cholinesterase inhibitors

| PP-15 |

A Novel Schiff base - based Fluorescent Chemosensor for Al³⁺ Ion Detection in Aqueous Solution

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Abstract

In acidic soils, aluminium is present in its solubilized form, Al³⁺, which is poisonous to both plants and animals. Al³⁺ detection and measurement are essential for biology as well as chemistry. A new Schiff base (SB) has been synthesized in this work. The interaction of SB with different metal ions has been studied using fluorescent spectra. The results show that SB is a highly selective and sensitive probe for Al³⁺ ions over other commonly coexisting metal ions in ethanol. A very obvious fluorescence enhancement effect was observed, and a turn-on ratio over 10000- fold was triggered with the addition of 10 equiv. of Al³⁺ ions. What is more, such fluorescent responses could be detected by the naked eye under a UV-lamp. The lowest detection limit for Al³⁺ was determined as 4.9 x 10⁻⁹ M. The complex solution (SB–Al³⁺) exhibited reversibility with EDTA. These results may be caused by the unique molecular structure.

Keywords: Schiff base, Fluorescent chemosensor, Al³⁺ Chemosensor

| PP-16 |

Biogenic Bandgap Engineering of Cu Infused TiO₂: Comparison Of Structural Evolution of Leaf and Seed Fusion Routes

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Abstract

The study here involves the synthesis of Copper infused TiO₂ influenced by a Fusion mix of five leaves(L1-1wt% and L2-0.5wt%) as well as five seeds(S1-1wt% and S2-0.5wt%) by Sol-Gel Method. The structural morphology is compared by SEM images with nanoparticle sizes ranging from 10-40nm. Elemental compositions are compared using EDAX data. The capping ability is estimated by determination of crystallite size by XRD with sizes varying from 6.4-7nm were identified. FTIR confirms the functional groups present. Bandgap engineering is compared using the UV Spectroscopy results giving a band gap drop of 2.2-2.85nm. Infusing copper with TiO₂ in the presence of these phytochemicals improve the conductivity by modifying the bandgap of TiO₂. Also the tropical changes here impart greater porosity and surface area to the newly formed material. The presence of green materials have significantly reduced the crystallite size thereby confirming the formation of smaller sized Anatase crystals.

Keywords: Fusion, Band gap Engineering, Phytochemicals, Capping

| PP-17 |

Synthesis, Characterisation and Pigment Studies of Cobalt-Doped Bismuth oxide (Bi_2O_3) Nanoparticles

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Abstract

Bismuth oxide (Bi_2O_3) is an important inorganic material due to its non-toxicity, favourable optical absorption in the visible region, high refractive index, and excellent chemical stability, making it suitable for pigment and optical applications. In the present work, undoped and cobalt-doped bismuth oxide nanoparticles with dopant concentrations of 1% and 5% Co are being synthesised via an oxalate precursor route using a wet chemical precipitation method, followed by thermal calcination. Cobalt doping is introduced to tailor the structural and optical properties of Bi_2O_3 by inducing lattice distortion and defect-related states. The prepared materials will be characterised using X-ray diffraction (XRD) to analyse phase formation and crystallite size, Fourier transform infrared spectroscopy (FTIR) to confirm metal-oxygen bonding, and UV-Visible diffuse reflectance spectroscopy to study optical absorption behaviour. Photoluminescence spectroscopy will be employed to investigate charge recombination characteristics, while surface morphology and particle size distribution will be examined using scanning electron microscopy (SEM). The cobalt-doped Bi_2O_3 samples are expected to exhibit noticeable colour variation and altered optical properties compared to undoped Bi_2O_3 , indicating their potential as eco-friendly inorganic pigments and functional materials. The study aims to explore the suitability of doped Bi_2O_3 nanoparticles for applications in pigments, coatings, photocatalysis, and optical devices.

Keywords: Bismuth oxide, Cobalt doping, Nanoparticles, Pigment properties, Optical properties

| PP-18 |

Structural, Spectroscopic and Optical Properties of LTF Single Crystals: Comparative Approach

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Abstract

By slow evaporation solution growth approach, L-tryptophan-fumaric acid monohydrate (LTF) crystals were formed. Using a single crystal X-ray diffraction (XRD) analysis, the crystal structure has been confirmed. Comparison of functional group arrangement of the grown crystal was studied through Fourier transform infrared (FTIR) and Fourier transform Raman spectrum (FT-Raman). Optical property of the as grown single crystal was analyzed by Ultraviolet-visible (UV-Vis) spectroscopy. Thermo Gravimetric Analysis (TG), Differentiated Thermal Analysis (DTA), and Differential Scanning Calorimetry were used to calculate thermal constancy and soppy point (DSC). By using the Kurtz-Perry powder method, the title compound's Second Harmonic Generation (SHG) was verified. Utilizing Gaussian 03 software, calculations for the first-order hyper polarizability particle Electrostatic Potential Map (MEP), and Frontier Molecular Orbital (FMO) was taken.

Keywords: Slow evaporation, Organic compound, Optical property, Vibrational studies, Thermal study and Density functional theory.

| PP-19 |

Synthesis and In-Silico Biological Evaluation of 3-Substituted 2-selenoquinoline derivatives to cyclooxygenase enzymes (COX-I and II)

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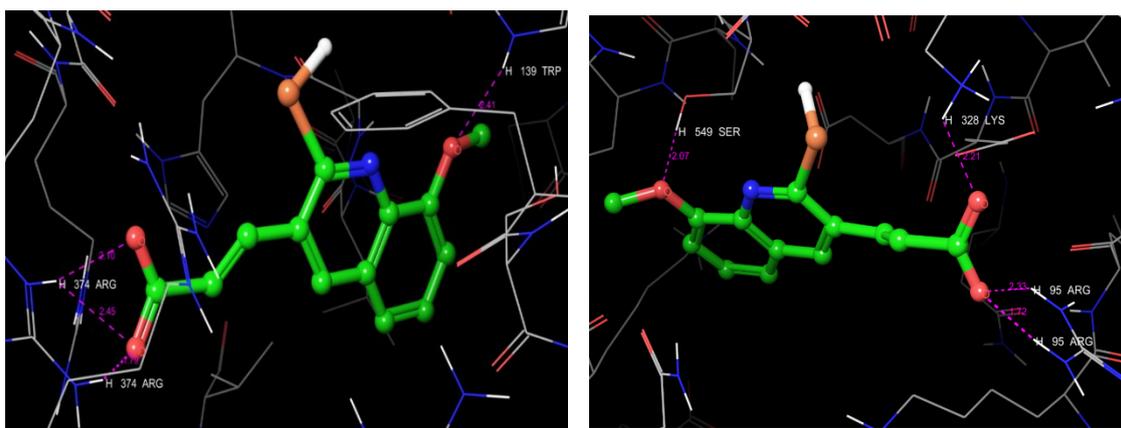
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Abstract

2-Chloro-3-formylquinoline derivatives were synthesized via the Vilsmeier–Haack reaction and subsequently transformed into selenoquinoline analogues using Na₂Se. The intermediates were further subjected to Knoevenagel condensation with various α,β -unsaturated carbonyl compounds to obtain a series of 3-substituted selenoquinoline derivatives. The synthesized compounds were structurally characterized by FT-IR, ¹H-NMR, ¹³C-NMR, and mass spectrometry. Biological evaluation was carried out to assess antibacterial and antioxidant activities, along with molecular modeling studies targeting COX-I and COX-II (cyclooxygenase enzymes) using the Schrödinger software. QSAR analysis indicated that 2-selenoquinoline-3-acrylic acid exhibited superior binding affinity, reflected by a favorable binding energy in terms of Glide score and Glide energy (−5.7, −41.65kcal/mol) with arginine and tryptophan residues in the active sites of COX-I and COX-II.

Keywords: Selenoquinolines, Antibacterial, Antioxidant assay, Molecular modeling, COX I & II.



| PP-20 |

Valorization of Bio-Litter into Cellulose Adsorbents for Lead (II) Water Treatment

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Abstract

Intensification of industrial activity, environment stress contributes to the significant rise of heavy metal pollution in water resources. Pollution due to malignant heavy metals such as lead, chromium, arsenic etc., has been tremendously focused on communal health. Lead pollution-potable water finds great threat by different sources like plating units, lead pipes etc., The present study evaluates the potentiality of Chemically Modified Cellulose Puree (CMCP) for sequestration of Pb (II) ions. Characterizations of loaded and unloaded puree were evaluated by FTIR, SEM and EDAX assay. Batch experimental studies were accomplished to assess the equilibration between the sorbate-sorbent through various operating factors viz., pH, dosage, time course, and initial concentration, influence of ions, co-ions and effect of temperature. The residual concentrations of the Pb²⁺ ions from aqueous solutions are examined by UV-Visible Spectrophotometer. The equilibrium data was appropriately fitted with Langmuir adsorption isotherm model.

Keywords: Chemically Modified Cellulose Puree, Lead, Batch Studies, Isotherms

| PP-21 |

Investigation of Strontium Ferrite Nanoparticles using Hydrothermal approach for Photocatalytic Degradation of Methylene Blue Dye

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Abstract

This study investigates the structural characteristics and photocatalytic performance of strontium ferrite ($\text{SrFe}_{12}\text{O}_{19}$) and cobalt-doped strontium ferrite nanoparticles synthesized via a hydrothermal technique. X-ray diffraction analysis revealed the formation of a single-phase hexagonal, with peak shifts indicating successful cobalt incorporation. Fourier-transform infrared spectroscopy confirmed the presence of characteristic Fe–O vibrations, while UV–Vis spectroscopy revealed a reduction in band gap energy upon cobalt doping, enhancing light absorption. Photoluminescence studies demonstrated suppressed electron–hole recombination in doped samples, contributing to improved photocatalytic performance. Scanning electron microscopy revealed agglomerated nanoparticles with near-spherical morphology, and thermo gravimetric analysis confirmed high thermal stability of the synthesized materials. The photocatalytic efficiency of the nanoparticles was assessed through the photo degradation of Methylene blue dye under visible light irradiation. Cobalt-doped strontium ferrite revealed superior photocatalytic activity compared to undoped $\text{SrFe}_{12}\text{O}_{19}$, attributed to enhanced charge carrier dynamics and improved optical absorption. These results indicate that cobalt -doped strontium ferrite nanoparticles hold significant potential for environmental application, especially in the photocatalytic removal of organic contaminants from the wastewater. This research contributes to the development of efficient and sustainable materials for addressing water pollution challenges.

Keywords: Strontium ferrite; Cobalt-doped ferrite; Hydrothermal synthesis; Photo catalysis; Methylene blue degradation

| PP-22 |

Ultrasmall N/S-doped Nb₂C MXene Quantum Dots as a Fluorescent “Turn-off” Platform for Sensitive Chloramphenicol Sensing in Food Samples

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Abstract

The development of a simple, aptamer-free, real-time fluorescence platform for the rapid and accurate detection of the essential antibiotic drug chloramphenicol (CPL) holds great promise for use in food, environmental, and clinical diagnostics. Here, we introduce a highly luminescent, bluish-green-emitting ultra-small N/S-co-doped Nb₂C MXene quantum dots (Nb₂C-MX QDs) synthesized through a hydrothermal process with glutathione as a nitrogen and sulfur dopant. These synthesized Nb₂C-MX QDs exhibit a strong fluorescence peak at 427 nm under 330 nm excitation, making them a straightforward fluorescent nano-label for CPL sensing. Leveraging the QDs' outstanding optical properties, the fluorescence peak of Nb₂C-MX QDs is significantly and dose-dependently quenched upon the addition of CPL antibiotic. This notable quenching effect results from the formation of non-fluorescent complexes between the Nb₂C-MX QDs and the CPL antibiotic, effectively triggering a "turn-off" fluorescence response. The proposed sensing platform has a detection limit of approximately 76.3 nM and exhibits excellent detection performance with a range of 20-240 μM. Importantly, interference tests confirm the system's high specificity, as CPL markedly suppresses the fluorescence signal of Nb₂C-MX QDs, while other common interferents, such as amino acids, biomolecules, and some antibiotics, do not affect the emission signal. Finally, the developed sensor was successfully applied to measure CPL levels in real samples, including tap water, drinking water, human blood and urine, and milk, achieving excellent recovery rates from 92.31% to 98.24%, underscoring its significant potential for practical, point-of-care diagnostics in environmental, food, and clinical settings.

Keywords: Antibiotic drug, Chloramphenicol, 2D MXene, Fluorescence quenching, Human serum sample, Urine sample, Milk samples

| PP-23 |

Synthesis, Structural Characterization and Biological Evaluation of New Nickel (II) Complexes Containing Coumarin based Schiff Bases

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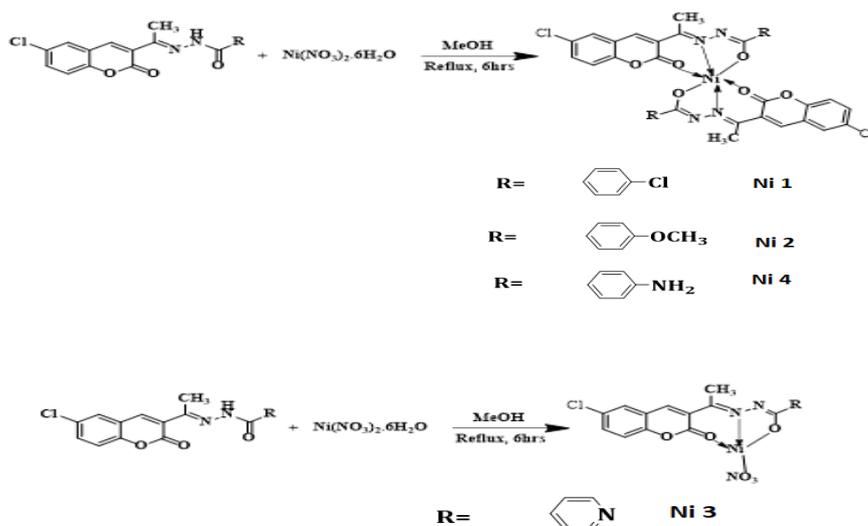
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Abstract

A set of 6-chloroacetyl coumarin appended hydrazones and their Nickel (II) complexes have synthesised and characterized by using various spectroscopic techniques such as IR, UV-Visible, ¹H NMR, and mass spectrometric techniques. Structural characterization of the complexes revealed the coordination of azomethine nitrogen, ring carbonyl oxygen and enolate oxygen atoms of the ligands to the nickel (II) ion and form the ML₂ type complexes (Scheme 1) in Ni 1, Ni 2 and Ni 4 complexes, whereas in complex Ni 3 the ligand coordinate as monobasic tridentate manner via azomethine nitrogen, ring carbonyl oxygen and enolate oxygen atoms to form four coordinated complex. The complexes are air-stable and soluble in most organic solvents. The compounds showed potent anti-cancer activity with MCF-7 and HeLa cells compared with standard drug cisplatin. Further their selectivity towards the cancer cells rather than normal cells was confirmed with HUVEC cells.

Keywords: Schiff bases, Coumarin, Nickel(II) complex, Anti-cancer studies.



| PP-24 |

Pigment Characteristics of Nickel Ferrite Powders

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Abstract

Ferrite-based pigments have much attention in near infrared (NIR)-reflective paints, conductive paint, and anti-corrosion coatings. Herein, nickel ferrite (NiFe₂O₄) pigment powder was synthesised by a two-step precipitation-thermal decomposition route. Metal (nickel/ferrous) oxalates were prepared by a precipitation method. In the second step, the as-formed nickel/ferrous oxalates were calcined at three different temperatures in a muffle furnace. The calcination temperature of nickel/ferrous oxalates was fixed by using thermo gravimetric analysis (TGA). The synthesis as-prepared NiFe₂O₄ samples were examined by Fourier transform infrared (FTIR), and UV-visible spectroscopic techniques. The presence of metal-oxygen (Fe-O/Ni-O) stretching vibrations were confirmed by observing characteristic FTIR bands. The d-d transition and ligand to metal charge transfer transitions were also noted in the UV-Visible spectra of NiFe₂O₄ samples. The chromaticity features of NiFe₂O₄ pigments were analysed by the CIE 1931 method (UV-visible spectrophotometer). The CIE x and CIE y coordinates were determined. The effect of calcination temperature on the pigment feature of NiFe₂O₄ powders have been assessed.

Keywords: Ferrite, NiFe₂O₄, Precipitation-thermal decomposition route, Pigments

| PP-25 |

Photo-Fenton-like Catalytic Property of Fe₂O₃/Bi₂O₃ Composite

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Abstract

In this paper, the facile synthesis of Iron (III) oxide (Fe₂O₃)/bismuth oxide (Bi₂O₃) composite photocatalyst has been reported. Ferrous oxalate and bismuth nitrate were used as metal precursors. The formation of Fe₂O₃ and Bi₂O₃ crystals were confirmed by powder X-ray diffraction analysis. The presence of Fe-O and Bi-O bonds (metal - oxygen) in Fe₂O₃/Bi₂O₃ composite was identified via a Fourier transform (FTIR) infrared spectroscopy. Fe₂O₃/Bi₂O₃ composite shows good absorption in the visible light region. Tauc plot was employed to calculate the band gap of Fe₂O₃/Bi₂O₃ composite. The photocatalytic properties of Fe₂O₃/Bi₂O₃ composite were examined by using hydrogen peroxide (H₂O₂)-mediated degradation of methylene blue (1×10⁻⁵ M, 100 ml) and Congo red (3×10⁻⁵ M, 100 ml) in water medium under visible light irradiation. For comparison, the photocatalytic experiments have also been conducted in the absence of H₂O₂. Fe₂O₃/Bi₂O₃ composite showed photocatalytic activity under the optimized experimental condition and thus it is expected to become a great catalyst in the photocatalytic treatment of dye effluents.

Keywords: Fe₂O₃/Bi₂O₃, Composite, Photocatalysis, H₂O₂, Methylene blue, Congo red.

| PP-26 |

Effect of ZnSrFe₂O₄ Content on Magnetic and Dielectric Properties of Poly(o-phenylenediamine)/ZnSrFe₂O₄ Nanocomposites

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Abstract

This study focuses on the synthesis and characterization of ZnSrFe₂O₄/poly (o-phenylenediamine) (ZnSrFe₂O₄/PoPD) nanoparticles and nanocomposites, designed to enhance the tremendous applications in various field. By Self-sustained exothermic method ZnSrFe₂O₄ nanoparticles were prepared and the nanocomposites were prepared by in situ polymerization of o-phenylenediamine in the presence of nanoparticles. ZnSrFe₂O₄ The structural, morphological and chemical characteristics of the nanocomposites were investigated using techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared (FTIR) spectroscopy confirming the successful incorporation of CuSrFe₂O₄ into the polymer matrix. Electrochemical analysis, including cyclic voltammetry (CV) and charge-discharge tests, revealed an improvement in the conductivity, stability and electrochemical performance of the nanocomposites when compared to the individual components. These results demonstrate that the ZnSrFe₂O₄/PoPD nanocomposites exhibit synergistic effects, where the conductive polymer enhances the charge transport properties and the ZnSrFe₂O₄ nanoparticles provide magnetic and catalytic benefits. This combination results in a versatile material suitable for a range of applications, including energy storage devices, sensors, and catalytic processes, offering a promising pathway for future material development in advanced technologies.

Keywords: Nanocomposites, PXRD, SEM, TEM, Dielectric constant, Thermal properties

| PP-27 |

Preparation, Electrical and Magnetic Properties of Poly (o-phenylenediamine)/CrSrFe₂O₄ Nanocomposites

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Abstract

This study focuses on the synthesis and characterization of CrSrFe₂O₄/poly (o-phenylenediamine) (CrSrFe₂O₄/PoPD) nanoparticles and nanocomposites, designed to enhance the tremendous applications in various field. By Self-sustained exothermic method CrSrFe₂O₄ nanoparticles were prepared and the nanocomposites were prepared by in situ polymerization of o-phenylenediamine in the presence of nanoparticles. The structural, morphological and chemical characteristics of the nanocomposites were investigated using techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier-transform infrared (FTIR) spectroscopy confirming the successful incorporation of CrSrFe₂O₄ into the polymer matrix. Electrochemical analysis, including cyclic voltammetry (CV) and charge-discharge tests, revealed an improvement in the conductivity, stability and electrochemical performance of the nanocomposites when compared to the individual components. These results demonstrate that the CrSrFe₂O₄/PoPD nanocomposites exhibit synergistic effects, where the conductive polymer enhances the charge transport properties and the CrSrFe₂O₄ nanoparticles provide magnetic and catalytic benefits. This combination results in a versatile material suitable for a range of applications, including energy storage devices, sensors, and catalytic processes, offering a promising pathway for future material development in advanced technologies.

Keywords: Nanocomposites, PXRD, SEM, TEM, Dielectric constant, Thermal properties

| PP-28 |

Synthesis, Structural, Magnetic and Electrical Characterization of Poly (o-phenylenediamine)/BaSrFe₂O₄ Nanocomposites

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Abstract

This study focuses on the synthesis and characterization of BaSrFe₂O₄/poly (o-phenylenediamine) (BaSrFe₂O₄/PoPD) nanoparticles and nanocomposites, designed to enhance the tremendous applications in various field. By Self-sustained exothermic method BaSrFe₂O₄ nanoparticles were prepared and the nanocomposites were prepared by in situ polymerization of o-phenylenediamine in the presence of nanoparticles. The structural, morphological and chemical characteristics of the nanocomposites were investigated using techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier-transform infrared (FTIR) spectroscopy confirming the successful incorporation of BaSrFe₂O₄ into the polymer matrix. Electrochemical analysis, including cyclic voltammetry (CV) and charge-discharge tests, revealed an improvement in the conductivity, stability and electrochemical performance of the nanocomposites when compared to the individual components. These results demonstrate that the BaSrFe₂O₄/PoPD nanocomposites exhibit synergistic effects, where the conductive polymer enhances the charge transport properties and the BaSrFe₂O₄ nanoparticles provide magnetic and catalytic benefits. This combination results in a versatile material suitable for a range of applications, including energy storage devices, sensors, and catalytic processes, offering a promising pathway for future material development in advanced technologies.

Keywords: Nanocomposites, PXRD, SEM, TEM, Dielectric constant, Thermal properties

| PP-29 |

Investigation of Magnetic and Dielectric Properties of Poly (o-phenylenediamine)/CuSrFe₂O₄ Nanocomposites

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Abstract

This work investigates the synthesis and properties of CuSrFe₂O₄/poly (o phenylenediamine) (CuSrFe₂O₄/PoPD) nanoparticles and nanocomposites, aiming to explore their potential in advanced functional applications. By self- sustained exothermic method CuSrFe₂O₄ nanoparticles were prepared and the nanocomposites were synthesized through the in-situ polymerization of o-phenylenediamine in the presence of CuSrFe₂O₄ nanoparticles. Characterization techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier-transform infrared (FTIR) spectroscopy were employed to confirm the successful formation of the nanocomposite structure. The electrochemical performance was assessed via cyclic voltammetry (CV) and charge-discharge tests showing notable improvements in conductivity, stability and charge storage capacity compared to individual CuSrFe₂O₄ and poly(o-phenylenediamine). The nanocomposites demonstrated a synergistic effect where the conductive polymer matrix and magnetic nanoparticles enhanced each other's properties making the material promising for applications in energy storage systems, sensors, electrical properties and environmental remediation. These findings suggest that CuSrFe₂O₄/PoPD nanocomposites have significant potential in multifunctional material design for next-generation technologies.

Keywords: PoPD, CuSrFe₂O₄, PXRD, SEM, TEM, Magnetic studies, Electrical studies.

| PP-30 |

Harnessing Cd-doped ZnO Nanoparticles for Solar and UV-C induced Azo Dyes Degradation and Broad-Spectrum Antibacterial Activity

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Abstract

Water pollution caused by the discharge of persistent organic dyes from industrial effluents represents a serious environmental and public health concern. These dyes are chemically stable, toxic, and resistant to conventional wastewater treatment processes, necessitating the development of efficient and sustainable remediation technologies. In this study, pure and cadmium-doped zinc oxide (Cd-ZnO) nanoparticles were synthesised, characterised, and evaluated as effective photocatalysts for environmental remediation applications. Cadmium doping was employed to enhance the photocatalytic and antibacterial performance of ZnO by tuning its band structure, improving light absorption, and promoting the generation of reactive oxygen species (ROS). The photocatalysts were synthesised via a simple chemical precipitation method and comprehensively characterised using XRD, FT-IR, Raman spectroscopy, FE-SEM, EDS, HR-TEM, XPS, UV-DRS, and photoluminescence techniques to investigate their structural, morphological, chemical, and optical properties. Photocatalytic degradation studies were conducted using two model azo dyes, Reactive Red 120 (RR120) and Acid Black 1 (AB1), under both UV-C irradiation and natural sunlight. Among the samples, 3 wt% Cd-ZnO exhibited superior photocatalytic performance, achieving nearly 100% degradation within 120–150 minutes, as supported by kinetic analyses. The practical applicability of the catalyst was further examined through reusability tests, pH variation studies, and catalyst dosage optimisation. Active species trapping experiments and GC-MS analysis were performed to elucidate the degradation mechanism and intermediates. Additionally, antibacterial activity against both Gram-positive and Gram-negative bacteria confirmed the multifunctional potential of Cd-ZnO for integrated wastewater treatment and microbial disinfection.

Keywords: Photocatalysis, Dye degradation, UV/Solar irradiation, Antibacterial activity, Environmental remediation

| PP-31 |

Zr-modified ZnO Nanoparticles: Optimized Photocatalytic Degradation and Antibacterial Efficiency for Pollution Control

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Abstract

Rapid urban expansion and industrial advancement have led to severe environmental pollution, particularly in water bodies contaminated with toxic dyes and harmful pathogens. Zinc oxide (ZnO) nanoparticles have been extensively researched for their photocatalytic and antibacterial properties. However, their efficiency is limited by rapid electron-hole recombination and poor light absorption. In this study, ZnO nanoparticles doped with zirconium (Zr) were synthesized to overcome these limitations. Structural, morphological, and optical analyses, including XRD, FT-IR, FT-Raman, PL, UV-DRS, XPS, FE-SEM, HR-TEM, and EDS confirmed the successful incorporation of Zr into ZnO lattice. This incorporation effectively reduced the band gap from 3.11 eV to 3.05 eV. This modification enhanced both light absorption and charge separation. Photocatalytic degradation tests using the azo dye such as Reactive Red 120 under UV-A and sunlight exposure demonstrated that 3 wt% Zr-doped ZnO achieved nearly 100 % degradation efficiency under both light sources. The intermediates were analysed by GC- MS analysis, and a suitable degradation pathway is proposed. Additionally, antibacterial assays towards *Pseudomonas aeruginosa*, *Bacillus subtilis*, *Staphylococcus aureus* and *Escherichia coli* showed a significant increase in bacterial inhibition with Zr-doped ZnO. These results indicate that Zr-doped ZnO nanoparticles are interesting candidates for environmental applications such as wastewater treatment and antimicrobial surface coatings.

Keywords: Zr-ZnO, UV-A light, Azo dye, Photocatalytic activity, Environmental remediation

| PP-32 |

Study of Magnetic and Electrical Properties of Poly (o- phenylenediamine/NiSrFe₂O₄) Nano Composites

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Abstract

This work investigates the synthesis and properties of NiSrFe₂O₄/poly (o-phenylenediamine) (NiSrFe₂O₄/PoPD) nanoparticles and nanocomposites, aiming to explore their potential in advanced functional applications. By self-sustained exothermic method NiSrFe₂O₄ nanoparticles were prepared and the nanocomposites were synthesized through the in-situ polymerization of o-phenylenediamine in the presence of NiSrFe₂O₄ nanoparticles. Characterization techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier-transform infrared (FTIR) spectroscopy were employed to confirm the successful formation of the nanocomposite structure. The electrochemical performance was assessed via cyclic voltammetry (CV) and charge-discharge tests showing notable improvements in conductivity, stability and charge storage capacity compared to individual NiSrFe₂O₄ and poly(o-phenylenediamine). The nanocomposites demonstrated a synergistic effect where the conductive polymer matrix and magnetic nanoparticles enhanced each other's properties making the material promising for applications in energy storage systems, sensors, electrical properties and environmental remediation. These findings suggest that NiSrFe₂O₄/PoPD nanocomposites have significant potential in multifunctional material design for next-generation technologies.

Keywords: PoPD, NiSrFe₂O₄, PXRD, SEM, TEM, Magnetic studies, Electrical studies

| PP-33 |

Investigation of Magnetic, Dielectric and Thermal Properties of Poly (o-phenylenediamine)/SrCuFe₂O₄ Nanocomposites

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Abstract

This study focuses on the synthesis and characterization of SrCuFe₂O₄/poly (o-phenylenediamine) (SrCuFe₂O₄/PoPD) nanoparticles and nanocomposites, designed to enhance the tremendous applications in various field. By Self-sustained exothermic method SrCuFe₂O₄ nanoparticles were prepared and the nanocomposites were prepared by in situ polymerization of o-phenylenediamine in the presence of CuSrFe₂O₄ nanoparticles. The structural, morphological and chemical characteristics of the nanocomposites were investigated using techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier-transform infrared (FTIR) spectroscopy confirming the successful incorporation of SrCuFe₂O₄ into the polymer matrix. Electrochemical analysis, including cyclic voltammetry (CV) and charge-discharge tests, revealed an improvement in the conductivity, stability and electrochemical performance of the nanocomposites when compared to the individual components. These results demonstrate that the SrCuFe₂O₄/PoPD nanocomposites exhibit synergistic effects, where the conductive polymer enhances the charge transport properties and the SrCuFe₂O₄ nanoparticles provide magnetic and catalytic benefits. This combination results in a versatile material suitable for a range of applications, including energy storage devices, sensors, and catalytic processes, offering a promising pathway for future material development in advanced technologies.

Keywords: Nanocomposites, PXRD, SEM, TEM, Dielectric constant, Thermal properties

| PP-34 |

Poly (o-Phenylenediamine)/CuCrFe₂O₄ Nanocomposites: Synthesis, Structural Characterization, Thermal, Magnetic and Electrical Properties

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Abstract

Novel o-phenylenediamine POPD/ CuCrFe₂O₄ with two different ratios of CuCrFe₂O₄ (10% and 25%) were synthesized by a renowned method of in-situ oxidative chemical polymerization. This composition of CuCrFe₂O₄ nanoparticles were prepared by auto self exothermic method. The following methods, Fourier - transform infrared spectrum (FTIR), UV spectrometer, scanning electron microscopy (SEM), Transmittance electron microscopy (TEM), X-ray diffraction (XRD), were used to analyze the structural, thermal and morphological properties of the nano particles and nanocomposites. The magnetic properties of both the nanoparticles and the nanocomposites were analyzed by Vibrating sample magnetometer (VSM). The visualization of the dielectric properties, were shown at different temperatures.

Keywords: CuCrFe₂O₄, PXRD, SEM, TEM, VSM, Thermal and Dielectric properties.

| PP-35 |

Synthesis, Structural, Electrical and Magnetic Properties of Poly (O-Phenylenediamine)/ BaCrFe₂O₄ Nanocomposites

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Abstract

BaCrFe₂O₄ Nano particles were prepared by self-exothermic method. Nano composites consisting o-phenylenediamine POPD/ BaCrFe₂O₄ with two different ratios of BaCrFe₂O₄ (10% and 25%) were synthesized by a renowned method of in-situ oxidative chemical polymerization. The following methods, Fourier - transform infrared spectrum (FTIR), UV spectrometer, scanning electron microscopy (SEM), Transmittance electron microscopy (TEM), X-ray diffraction (XRD), were used to analyze the structural, thermal and morphological properties of the nano particles and nanocomposites. The magnetic properties of both the nanoparticles and the nanocomposites were analyzed by Vibrating sample magnetometer (VSM). The visualization of the dielectric properties, were shown at different temperatures.

Keywords: BaCrFe₂O₄, FT-IR, PXRD, SEM, TEM, Electrical and Magnetic properties.

| PP-36 |

Oxygen-Rich Biomass-Derived Carbon Dots for Sensitive Fluorescent Detection of Ciprofloxacin in Water

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Abstract

Oxygen-rich carbon dots (O-CDs) were prepared from citron peel biomass using an environmentally benign hydrothermal method, resulting in well-dispersed fluorescent nanoparticles with an average size of 3-5 nm. FTIR and XPS characterizations revealed a high density of oxygen-containing surface functionalities, including carboxyl, hydroxyl, and carbonyl groups, imparting enhanced hydrophilicity and strong binding affinity toward ciprofloxacin (CIP). The synthesized O-CDs exhibited stable blue fluorescence with a maximum emission at 450 nm upon excitation at 365 nm and showed excellent photostability and water solubility, with a quantum yield of 15.2%. The presence of CIP induced an efficient fluorescence quenching response, primarily governed by static complex formation combined with the inner filter effect, as confirmed by absorption spectral overlap and Stern-Volmer analysis. Under optimized sensing conditions, the fluorescence probe displayed a linear response over a CIP concentration range of 1.0–60 μM , with a detection limit of 0.21 μM . The sensing system demonstrated high selectivity for CIP against various coexisting metal ions and structurally related antibiotics, attributed to strong hydrogen bonding and π - π interactions between CIP molecules and the oxygen-rich CD surface. The practical feasibility of the method was validated through successful determination of CIP in tap and river water samples, achieving satisfactory recoveries between 93.4% and 101.8%. This study highlights the potential of oxygen-rich, citron-derived carbon dots as a sustainable and effective fluorescent platform for monitoring ciprofloxacin contamination in aquatic environments.

Keywords: Oxygen-rich carbon dot, Citron-derived biomass, Ciprofloxacin detection, Fluorescent sensing, Environmental water analysis.

| PP-37 |

Nitrogen-Phosphorus Co-Doped Amino-Rich Biomass-Derived Carbon Dots as Green Fluorescent Probes for Malathion Detection

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Abstract

The extensive use of the organophosphate pesticide malathion in agricultural practices has raised serious concerns regarding food safety and environmental contamination, creating an urgent demand for simple, rapid, and sensitive analytical methods. This study aims to develop a green, single-emission fluorescent probe for malathion detection using nitrogen-phosphorus co-doped, amino-rich rice-husk-derived carbon dots (N,P-RH-CDs). The N,P-RH-CDs were synthesized via a sustainable hydrothermal route and characterized by abundant surface functional groups, including amino ($-\text{NH}_2$), hydroxyl ($-\text{OH}$), carboxyl ($-\text{COOH}$), and phosphate-related ($\text{P}-\text{O}/\text{P}=\text{O}$) moieties. These features provide strong blue fluorescence, excellent water dispersibility, and enhanced affinity toward malathion molecules. The sensing mechanism is based on concentration-dependent fluorescence quenching induced by photoinduced electron transfer and inner filter effects, facilitated by hydrogen bonding and electrostatic interactions between malathion and the functionalized carbon dot surface. Under optimized conditions, the sensor exhibits a linear detection range of 0.02–15.0 μM with a low limit of detection of 5.1 nM. The probe demonstrates high selectivity toward malathion in the presence of other pesticides, inorganic ions, and organic interferents. Practical applicability was validated through the analysis of spiked food and environmental water samples, yielding recoveries of 95.0–104.6% with relative standard deviations below 5%. This work highlights the effectiveness of heteroatom-doped, biomass-derived carbon dots as environmentally friendly and cost-effective fluorescent probes for pesticide residue monitoring and food safety assessment.

Keywords: Nitrogen-phosphorus co-doped carbon dots, Amino-rich surface functionalization, Fluorescent sensing, Malathion detection, Organophosphate pesticides, Biomass-derived nanomaterials

| PP-38 |

A Review on Green Synthesis of ZnO Nanoparticles - An Ecofriendly Approach

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Abstract

Nanotechnology focuses on creating and utilizing materials at an extremely small scale, where particles possess a significantly larger surface area compared to their overall size. This unique characteristic gives them specialized properties. Zinc oxide nanoparticles (ZnO NPs) have garnered significant research interest due to their wide range of potential applications, including fighting bacteria and fungi, managing diabetes, reducing inflammation, promoting wound healing, combating oxidative stress, and manipulating light. Traditional methods of producing these nanoparticles often involve harsh chemicals and extreme conditions, which can be harmful. To address these concerns, environmentally friendly approaches have emerged, utilizing living organisms like plants, fungi, bacteria, and algae. This paper offers a thorough examination of the various methods used to create and analyze ZnO NPs through these biological, "green" synthesis techniques.

Keywords: Zinc oxide nanoparticles; Biosynthesis plant; Microbes; Algae

| PP-39 |

Synthesis, Structural Characterization, Thermal, Magnetic and Electrical Properties of $\text{CuCrFe}_2\text{O}_4$: Nanocomposites

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Abstract

Novel o-phenylenediamine POPD/ $\text{CuCrFe}_2\text{O}_4$ with two different ratios of $\text{CuCrFe}_2\text{O}_4$ (10% and 25%) were synthesized by a renowned method of in-situ oxidative chemical polymerization. This composition of $\text{CuCrFe}_2\text{O}_4$ nanoparticles were prepared by auto self exothermic method. The following methods, Fourier - transform infrared spectrum (FTIR), UV spectrometer, scanning electron microscopy (SEM), Transmittance electron microscopy (TEM), X-ray diffraction (XRD), were used to analyze the structural, thermal and morphological properties of the nano particles and nanocomposites. The magnetic properties of both the nanoparticles and the nanocomposites were analyzed by Vibrating sample magnetometer (VSM). The visualization of the dielectric properties, were shown at different temperatures.

Keywords: $\text{CuCrFe}_2\text{O}_4$, PXRD, SEM, TEM, VSM, Thermal and Dielectric properties.

| PP-40 |

Electrical and Magnetic Properties of Poly (O-Phenylenediamine)/ CrCoFe₂O₄ Nanocomposites

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Abstract

In this study, nanocomposites consisting o-phenylenediamine POPD/ CrCOFe₂O₄ with two different ratios of CrCOFe₂O₄ (10% and 25%) were synthesized by a renowned method of in-situ oxidative chemical polymerization. This composition of CrCOFe₂O₄ nanoparticles were prepared by auto combustion method. The following methods, Fourier - transform infrared spectrum (FTIR), UV spectrometer, scanning electron microscopy (SEM), Transmittance electron microscopy (TEM), X-ray diffraction (XRD), were used to analyze the structural, thermal and morphological properties of the nano particles and nanocomposites. The magnetic properties of both the nanoparticles and the nanocomposites were analyzed by Vibrating sample magnetometer (VSM). The visualization of the dielectric properties, were shown at different temperatures.

Keywords: Nanocomposites, FT-IR, SEM, TEM, Magnetic and Dielectric properties.

| PP-41 |

Green Synthesis of Lead-Tin Metal Oxide Nanoparticles using Euphorbia Hirta Plant Extract

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Abstract

Most researchers have traditionally focused on synthesizing nanoparticles using conventional chemical methods, which are often expensive, complex, and environmentally hazardous. In the present study, a simple, cost-effective, and eco-friendly green synthesis method was employed for the preparation of lead oxide nanoparticles (Pb-Sn MONPs) using Euphorbia Hirta plant extract. The extract of Euphorbia hirta served as a natural reducing and stabilizing (capping) agent in the synthesis process. Lead nitrate and tin chloride were used as bimetallic precursor compounds for the formation of Pb-Sn MONPs. Upon treatment of the metal precursors with the plant extract, stable lead-tin metal oxide nanoparticles were successfully formed. The synthesized Pb-Sn MONPs were characterized using UV–Visible spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), X-ray diffraction (XRD), and Energy Dispersive X ray Analysis (EDAX) to confirm their formation, crystalline nature, morphology, and elemental composition. The synthesized Pb-Sn MONPs exhibited notable Antioxidant studies are carried out to evaluate the ability of a substance to neutralize harmful free radicals in the body and antimicrobial activity against selected pathogenic bacterial strains. Additionally, their photocatalytic efficiency was evaluated through the degradation of organic dye under UV light irradiation, demonstrating their potential application in environmental remediation. This green synthesis approach highlights an economical, sustainable, and efficient method for producing Pb-Sn MONPs with promising biomedical and environmental applications.

Keywords: Green synthesis, Euphorbiaop; Hirta, Pb-Sn metal oxides, XRD, EDAX, Antioxidant

| PP-42 |

Sulfur-Doped Quantum Dots Integrated Fluorescent Sensor for Ultra-Sensitive Detection of Malathion Pesticide in Food Samples

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Abstract

The extensive use of organophosphorus pesticides such as malathion in agricultural practices has raised serious concerns regarding food safety and human health due to its high toxicity, environmental persistence, and accumulation at trace concentrations. In this work, sulfur-doped quantum dots (SQDs) were synthesized via a facile hydrothermal route and subsequently coupled with graphitic carbon nitride (g-C₃N₄) to construct a highly sensitive fluorescent nanosensor for malathion detection in complex food matrices. Sulfur doping introduces abundant surface defects and electron-rich active sites, significantly enhancing photoluminescence intensity and interfacial charge transfer. The resulting SQDs@g-C₃N₄ nanocomposite exhibits strong fluorescence emission, excellent photostability, and selective affinity toward malathion molecules, leading to pronounced fluorescence quenching through a combined static quenching and inner filter effect mechanism. Under optimized sensing conditions, the sensor demonstrates a wide linear response range from 10 to 120 μM, with an ultralow limit of detection of 0.02 μM, surpassing many reported fluorescent and chromatographic methods. High selectivity is achieved in the presence of common coexisting pesticides, metal ions, and food constituents. The practical applicability of the sensor is validated through the accurate determination of malathion in real food samples (vegetables and fruits), yielding satisfactory recoveries of 94.2–103.6% and relative standard deviations below 5%. This study highlights sulfur-doped quantum dot-based fluorescent nanoprobe as cost-effective, rapid, and reliable platforms for on-site pesticide residue monitoring and advanced food safety analysis.

Keywords: Sulfur-doped quantum dots, Malathion detection, Fluorescent nanosensor, Food safety analysis, Graphitic carbon nitride composite, Trace pesticide sensing.

| PP-43 |

Synthesis, Characterization and Environmental Application of CoSrFe₂O₄/Poly O-phenylenediamine Nanocomposites

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Abstract

This work investigates the synthesis and properties of CoSrFe₂O₄/poly (o-phenylenediamine) (CoSrFe₂O₄/PoPD) nanoparticles and nanocomposites, aiming to explore their potential in advanced functional applications. By self-sustained exothermic method CoSrFe₂O₄ nanoparticles were prepared and the nanocomposites were synthesized through the in-situ polymerization of o-phenylenediamine in the presence of CoSrFe₂O₄ nanoparticles. Characterization techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier-transform infrared (FTIR) spectroscopy were employed to confirm the successful formation of the nanocomposite structure. The electrochemical performance was assessed via cyclic voltammetry (CV) and charge-discharge tests showing notable improvements in conductivity, stability and charge storage capacity compared to individual CoSrFe₂O₄ and poly (o-phenylenediamine). The nanocomposites demonstrated a synergistic effect where the conductive polymer matrix and magnetic nanoparticles enhanced each other's properties making the material promising for applications in energy storage systems, sensors, electrical properties and environmental remediation. These findings suggest that CoSrFe₂O₄/PoPD nanocomposites have significant potential in multifunctional material design for next-generation technologies.

Keywords: PoPD, CoSrFe₂O₄, PXRD, SEM, TEM, Magnetic studies, Electrical studies

| PP-44 |

Boron-Doped Carbon Dots as Visible Light Responsive Nanocatalysts for Efficient Photocatalytic Degradation of Ciprofloxacin in Aqueous Systems

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Abstract

The increasing occurrence of antibiotic contaminants such as ciprofloxacin (CIP) in aquatic environments has become a major global concern due to their chemical persistence, contribution to antimicrobial resistance, and detrimental ecological effects. In this study, boron-doped carbon dots (B-CDs) were synthesized via a facile hydrothermal method and employed as efficient metal-free visible-light photo catalysts for the degradation of CIP in aqueous systems. Boron heteroatom incorporation induces abundant surface defects and electron-deficient sites, effectively narrowing the band gap, enhancing visible-light absorption, and promoting the separation and migration of photo-generated charge carriers. Under visible-light irradiation ($\lambda > 420$ nm), the B-CDs achieve a ciprofloxacin degradation efficiency exceeding 90% within 60 min, which is markedly higher than that of undoped carbon dots under identical conditions. Kinetic analysis reveals that the photocatalytic degradation follows a pseudo-first-order reaction model, with an apparent rate constant approximately 2.3 times higher than that of pristine CDs. Reactive species trapping experiments and electron spin resonance measurements confirm that hydroxyl radicals ($\bullet\text{OH}$) and superoxide radicals ($\bullet\text{O}_2^-$) are the dominant reactive oxygen species responsible for CIP oxidation, while photo-generated holes play a secondary role. The B-CDs exhibit excellent photochemical stability and reusability, retaining more than 85% of their initial catalytic activity after five consecutive cycles. This work demonstrates that boron-doped carbon dots represent a sustainable and environmentally benign nanocatalyst for antibiotic degradation and provides valuable insights into heteroatom-engineered carbon dots for advanced photocatalytic water treatment applications.

Keywords: Boron-doped carbon dots, Ciprofloxacin degradation, Visible light photocatalysis, Reactive oxygen species, Metal-free nanocatalyst, Water remediation.

| PP-45 |

Synthesis of Anticancer Agents: Molecular Docking and ADME Studies of New Hydropyrimidine Linked Amide-Pyridine Derivatives

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Abstract

To develop novel hydropyrimidine linked amide-pyridine hybrids as anticancer agents. An array of molecular hybrids **6a-6n** has been synthesized and evaluated for their *in vitro* cytotoxicity against breast (MCF-7, MDA-MB-231), pancreatic (AsPC-1, BxPC-3, SW1990), and normal cell lines (HEK-293, MRC-5, MCF-10A). Further, *in silico* absorption, distribution, metabolism, and excretion (ADME), docking, molecular dynamics (MD) simulation and density functional theory (DFT) studies of potent hybrids were executed. Hybrids **6i** and **6l** showed enhanced activity against breast cancer cells with IC₅₀ between 6.15±0.39 and 41.82±4.94 μM while **6m** exhibited enhanced activity against both breast and pancreatic cancer cells with IC₅₀ between 8.72±0.64 and 36.24±3.34 μM (p<0.05, three independent biological replicates). Against breast cancer cells, **6m** displayed ~3-fold superior activity than 5-fluorouracil while against pancreatic cancer cells, it exhibited comparable to superior activity. Further, **6m** selectively targets cancer cells over normal cells considerably, binds well with thymidylate synthase (-8.8 kcal.mol⁻¹), and forms stable complex as revealed from docking and MD simulation. ADME analysis proposes favourable features for good oral bioavailability. This study ascertains **6m** as promising lead for further biological evaluation and structural optimization towards the development of potential anticancer agents against pancreatic and breast cancers.

Keywords: Hydropyrimidine, *In silico* analysis, Cancer, Thymidylate synthase, Cytotoxicity

| PP-46 |

Chitosan Integrated CuAl LDH: A Sunlight Competent and Recoverable Photocatalyst for Nitrofurantoin Degradation

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Abstract

The persistent presence of pharmaceutical contaminants like nitrofurantoin (NFT) in aquatic environments poses a significant challenge to conventional water treatment technologies. In the present investigation, a CuAl layered double hydroxide (LDH) as well as its chitosan (CH)-integrated composite were synthesized, and their utilities as visible-light-driven photocatalysts for the effective degradation of nitrofurantoin (NFT) were evaluated. The structural/morphological features of the thus synthesized CuAl LDH and chitosan-integrated CuAl LDH composite, hereafter referred to as CuAl LDH:CH, were established through FT-IR, XRD, SEM, EDX, TEM, DRS-UV and XPS analyses. The results of optimization studies imply that the composite synthesized with CuAl LDH and chitosan (10:3, respectively) at pH 9 displayed enhanced photocatalytic efficiency, achieving ~96% degradation of NFT within 120 minutes under direct sunlight. This represents a ~30% improvement over pristine CuAl LDH. The incorporation of chitosan, a biopolymer rich in hydroxyl and amine groups, contributes significantly to surface dispersion, active site availability, and charge separation efficiency, resulting in superior visible-light photocatalytic performance. Further, the composite is stable and demonstrated commendable reusability over five cycles with no substantial decline in efficiency. The results indicate that the CuAl LDH:CH is a proficient and justifiable photocatalyst for the effective removal of NFT, a pharmaceutical pollutant, under direct sunlight.

Keywords: Layered double hydroxide, Copper–aluminium LDH, Chitosan-integrated composite, Visible-light photocatalysis, Nitrofurantoin degradation.

| PP-47 |

Plant-Based Synthesis of Lead-Tin oxide nanoparticles using *Euphorbia Hirta* plant extract

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Abstract

Most researchers have traditionally focused on synthesizing nanoparticles using conventional chemical methods, which are often expensive, complex, and environmentally hazardous. In the present study, a simple, cost-effective, and eco-friendly green synthesis method was employed for the preparation of lead oxide nanoparticles (Pb-Sn MONPs) using *Euphorbia Hirta* plant extract. The extract of *Euphorbia hirta* served as a natural reducing and stabilizing (capping) agent in the synthesis process. Lead nitrate and tin chloride were used as bimetallic precursor compounds for the formation of Pb-Sn MONPs. Upon treatment of the metal precursors with the plant extract, stable lead-tin metal oxide nanoparticles were successfully formed. The synthesized Pb-Sn MONPs were characterized using UV–Visible spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), X-ray diffraction (XRD), and Energy Dispersive X-ray Analysis (EDAX) to confirm their formation, crystalline nature, morphology, and elemental composition. The synthesized Pb-Sn MONPs exhibited notable Antioxidant studies are carried out to evaluate the ability of a substance to neutralize harmful free radicals in the body and antimicrobial activity against selected pathogenic bacterial strains. Additionally, their photocatalytic efficiency was evaluated through the degradation of organic dye under UV light irradiation, demonstrating their potential application in environmental remediation. This green synthesis approach highlights an economical, sustainable, and efficient method for producing Pb-Sn MONPs with promising biomedical and environmental applications.

Keywords: Green synthesis, *Euphorbia*; *Hirta*, Pb-Sn metal oxides, XRD, EDAX, Antioxidant.

| PP-48 |

Green Synthesis of Silver-Ion-Embedded Chitosan–PVA Nanocomposite Films Using *Leucas aspera* Leaf Extract for Antimicrobial Food Packaging Applications

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Abstract

The superior film-forming capabilities, biodegradability, and environmental compatibility of biopolymer-based nanocomposite films have made them effective and sustainable substitutes for traditional plastic packaging. Industrial and institutional research centers are interested in developing new food packaging films that use biodegradable materials like polyvinyl alcohol, herbal extracts, and food byproducts like chitosan. In this study, solution casting was used to create biodegradable films from chitosan and poly (vinyl alcohol) (PVA) matrices that were plasticized with glycerol and reinforced with silver ions reduced from *Leucas aspera* leaves extract. The solvent-cast films were conditioned in molds and refrigerated for 1 h and were allowed to dry for 48 hours at room temperature. FTIR and visible spectroscopy, water sorption, mechanical tests were used to characterize the prepared films. Measurements of antimicrobial activity against pathogen microorganisms were conducted to test the microbial activity of the film. The basic research showed that bio-based films produced increased the shelf life of the food and suggested that they could be utilized as innovative active food packaging materials.

Keywords: Chitosan, PVA, Bioactive film, Food packaging, Antimicrobial activity.

| PP-49 |

Development of Eco-Friendly Chitosan–PVA Based Nanocomposite Film Incorporated with Silver Ions for Antimicrobial Food Packaging Applications

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Abstract

Biopolymer-based nanocomposite films have emerged as sustainable and efficient alternatives to conventional plastic packaging due to their excellent film-forming abilities, biodegradability, and environmental compatibility. The use of biodegradable materials such as polyvinyl alcohol, herbal extracts and food byproducts such as chitosan to develop novel food packaging films attracts the interest of industrial and institutional research centers. In this research work, chitosan and poly (vinyl alcohol) (PVA) matrices plasticized with glycerol and reinforced with silver ions reduced using *Phyllanthus emblica* fruit extract and the biodegradable films were developed using solution casting technique. The solvent-cast films were conditioned in molds and refrigerated for 1 h, followed by drying at ambient temperature for 48 h. The prepared films were characterized by FTIR and visible spectroscopy, water sorption and mechanical measurements. Antimicrobial activity measurements were carried out against pathogen microorganisms. Overall, the results indicated that the use of the bio-based developed films led to an extension of food shelf life and could be used as novel active food packaging materials.

Keywords: chitosan, PVA, bioactive film, food packaging, antimicrobial activity

| PP-50 |

Fluorescent Detection of Carbamate Pesticides Using Biomass-Derived Nitrogen–Sulfur Co-Doped Carbon Dot@ZnO Nanocomposites

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Abstract

The widespread application of carbamate pesticides in agriculture has raised significant concerns regarding food safety and environmental contamination, necessitating the development of simple, rapid, and sensitive analytical methods. The objective of this study is to develop a green, single-emission fluorescent sensing platform for carbamate pesticide detection using biomass-derived nitrogen–sulfur co-doped carbon dot@ZnO (N,S-CD@ZnO) nanocomposites. Nitrogen–sulfur co-doped carbon dots were synthesized via a sustainable hydrothermal route using biomass precursors and subsequently coupled with ZnO nanoparticles to form a functional nanocomposite. Heteroatom doping introduces abundant –NH₂, –OH, –COOH, and –C–S– surface functional groups, enhances fluorescence emission, and modulates the electronic structure of carbon dots, thereby promoting efficient photoinduced electron transfer interactions with carbamate molecules. Upon exposure to carbamate pesticides, the fluorescence intensity of the N,S-CD@ZnO nanocomposite exhibits a concentration-dependent quenching response, enabling direct quantitative detection without the need for microfluidic devices or ratiometric signal processing. Under optimized conditions, the sensor demonstrates a linear detection range of 0.05–20.0 μM with a low limit of detection of 12 nM. The sensing platform shows excellent selectivity in the presence of common interfering ions, pesticides, and organic compounds. Practical applicability was validated through the analysis of real food samples, achieving recoveries of 94.1–105.3% with relative standard deviations below 5%. This work demonstrates the synergistic role of heteroatom doping and nanocomposite formation in developing cost-effective and environmentally friendly fluorescent probes for pesticide monitoring and food safety assessment.

Keywords: Nitrogen–sulfur co-doped carbon dots, Fluorescent sensing, Carbamate pesticides, ZnO nanocomposites, Food safety monitoring, Biomass-derived nanomaterials

| PP-51 |

Design and Fabrication of CuMoO₄/NiO as an Advanced Electrode for Hybrid Supercapacitors

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Abstract

In this present report, copper molybdate/nickel oxide (CuMoO₄/NiO) nanocomposites were successfully synthesised using a simple hydrothermal process. Structural analysis was proved that the formation of CuMoO₄/NiO nanocomposites. Morphological investigations were performed by SEM and TEM analysis and was confirmed the nano-spherical structure of the samples. Electrochemical studies were carried out and results showed that the optimised CuMoO₄/NiO electrode have a high specific capacitance of 700 F g⁻¹ at 1 A g⁻¹, which is greater than that of pristine CuMoO₄ (170 F g⁻¹). At the current density 5 A g⁻¹, the electrode demonstrated outstanding cycling stability by retaining 88% of its original capacitance after 5000 charge-discharge cycles. Additionally, at a current density of 1 A g⁻¹, it demonstrated good rate capability with 78% capacitance retention. From the above results, CuMoO₄/NiO nanocomposite show as promise electrode materials for high-performance supercapacitors in the future.

Keywords: CuMoO₄/NiO, Hydrothermal, Cyclic stability, Supercapacitor

| PP-52 |

Cobalt vanadate anchored on reduced graphene oxide: A high-performance electrode material for supercapacitors

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Abstract

Supercapacitors (SCs) have now been identified as potential power sources for efficient energy storage device applications. Hierarchical Cobalt Vanadium Oxide Nanoparticles (CVO) anchored on Graphene oxide Nanosheets (CVO-R) have been synthesized using a scalable and cost-effective hydrothermal method. The XRD analysis confirmed the phase composition of the prepared NCs. Furthermore, these CVO NPs were embedded in a continuous framework of graphene nanosheets, which led to the formation of a short path for ion transfer at the interface of the electrode and electrolyte, resulting in enhanced electrochemical properties. Working electrodes of COV NPs and COV-R NCs were fabricated and used their supercapacitor performances were tested with an aqueous KOH electrolyte. At 1 A g⁻¹, the composite showed high specific capacitance of 800 Fg⁻¹. It is indicative of superior electrochemical properties compared to a COV NPs. At 89.8% capacitance retention after 10,000 cycles, the composite has improved stability while retaining its superior rate capability. The observed findings underscore the strong potential of the CVO-R electrode for deployment in next-generation energy storage technologies.

Keywords: Cobalt vanadate, Hydrothermal, Supercapacitor, Stability.

| PP-53 |

Rapid Portable Detection of Chemical Warfare Agent Mimic Diethyl Chlorophosphate (DCP) using a Rhodamine-Quinoline Conjugated Probe with Fluorescent “Turn-on” and Chromogenic Responses, and Cancer Cell Imaging

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Abstract

Quantification of highly toxic nerve agents is seriously firm their deep health risks and potential for catastrophic consequences, highlighting the necessity for quick, reliable, and on-site sensing platforms. In this study, we present a portable, high-performance sensor specifically engineered for diethyl chlorophosphate (DCP), designed to deliver ultra-fast response, operational simplicity, and robust applicability in on-site scenarios. To detect DCP, we have developed the (*Z*)-2-(((6,8-dimethyl-2-oxo-1,2-dihydroquinolin-3-yl) methylene) amino)-3',6'-bis(ethylamino)-2',7'-dimethylspiro[isoinoline-1,9'-xanthen]-3-one (**RDE**) via a simple condensation reaction between the rhodamine hydrazide and 6,8-dimethyl-2-oxo-1,2-dihydroquinoline-3-carbaldehyde. The collected **RDE** molecule was successfully characterized by analytical spectroscopic techniques and a single-crystal X-ray diffraction analysis. Upon the injection of DCP into the **RDE** solution, the fluorescence signal at 598 nm increased by approximately 27-fold, indicating a strong fluorescence “turn-on” response. Interaction between DCP and **RDE** induced observable chromogenic changes, shifting from pale yellow to pink under daylight and from colorless to yellow emissive under UV light illumination. The xanthenyl moiety within the probe **RDE** serves as a reactive recognition unit, facilitating rapid interaction with DCP and enabling fluorescence signal generation within one minute, highlighting the sensor’s ultrafast response kinetics. Portable platforms, including paper strip-based test kits and smartphone-assisted RGB colorimetric analysis, were employed to evaluate the practical applicability of our developed **RDE** sensor for rapid, on-site detection of DCP. These portable approaches enable visual identification and semi-quantitative analysis of DCP, significantly reducing instrumentation costs, accelerating response times, and simplifying operational procedures, thereby demonstrating the sensor’s field-deployable utility and real-world applicability. Additionally, the developed receptor **RDE** was used to detect DCP in cancer cell imaging.

Keywords: Nerve agents, Smartphone, Paper strip test kit, Diethyl chlorophosphate, Rhodamine based receptor, Xanthenyl moiety

| PP-54 |

Conducting Bimetallic MOF Derived Nitride: A Unique Pathway for the Transformation of Amorphous to Metallic MOF

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Abstract

Bimetallic metal organic frameworks (MOFs) are considered as effective materials with abundant active metal sites and thus offers selective determination of target analysts. However, bimetallic MOF exhibited poor conductivity. Herein, in the present work a new pathway for the transformation of bimetallic MOF obtained via terephthalic acid as an organic linker has been transformed into conducting MOF. CoNi-MOF derived nitride (CoNiN) enhances electrical conductivity, surface area, and electrocatalytic activity and the obtained CoNiN coated on screen printed electrode (SPE) demonstrates exceptional performance for adenine and guanine oxidation, achieving high sensitivity ($0.4 \mu\text{A}/\mu\text{M}/\text{cm}^2$) & ($0.51 \mu\text{A}/\mu\text{M}/\text{cm}^2$), a low detection limit ($0.02 \mu\text{M}$ & $0.03 \mu\text{M}$) with a broad linear range ($0.1\text{--}180 \mu\text{M}$). Additionally, CoNiN exhibits excellent selectivity, stability, reproducibility, and practical applicability in detecting purines in real paracetamol tablet samples.

Keywords: CoNi-Bimetallic MOF, CoNiN bimetallic nitride, Electrochemical sensor, Adenine and guanine.

| PP-55 |

Thermal Synthesis of Fe₂O₃/ZnFe₂O₄ Composite Photocatalyst

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Abstract

Iron (III) oxides (Fe₂O₃) composites were reported for their photocatalytic performance than the pure Fe₂O₃. It is, due to improved photo-charge separation. In this research work Fe₂O₃/ZnFe₂O₄ was synthesized through thermal process. Zn (10%) doped Fe₃O₄ was used as a precursor to obtain Fe₂O₃ / ZnFe₂O₄ composite. Zn-doped Fe₃O₄ was synthesised by a coprecipitation method. The synthesized Fe₂O₃/ZnFe₂O₄ composite characterized by powder X-ray Diffraction (XRD), Fourier transform infrared (FT-IR) and UV-Visible spectroscopy. XRD analysis confirms the presence of diffraction peaks due to individual Fe₂O₃ and ZnFe₂O₄ components. The metal-oxygen (Fe-O/Zn-O) stretching vibration were also detected in the FTIR spectrum. When compared pure Fe₂O₃, the FTIR peak position of Fe-O is slightly altered. DRS UV-Visible spectroscopy was applied to study the optical property of Fe₂O₃/ZnFe₂O₄ composite. Characteristic absorption peaks were noted for Fe₂O₃/ZnFe₂O₄ composite, whereas the optical band gap value was estimated by using Tauc plot. Fe₂O₃/ZnFe₂O₄ nanocomposite was tested as a photocatalyst for degradation of Congo red and methylene blue.

Keywords: Fe₂O₃, Thermal synthesis, Photocatalysis, Methylene blue, Congo red, Water treatment.

| PP-56 |

Polymer Electrolyte Membrane for Fuel cell Applications

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Abstract

One of the promising and environmental friendly energy source - Fuel cell, It has great potential application in the areas from portable device to heavy power requirements. Polymer electrolyte membranes (PEMs) are the heart of fuel cell technology, controlling ion transport, electrochemical performance, and system durability. Among the various PEM materials, sulfonated polymers have emerged as highly promising candidates due to their strong proton conductivity, tunable structure, and cost-effective processing. Sulfonated polymers have emerged as promising alternatives to perfluorosulfonic acid membranes for proton exchange membrane fuel cell (PEMFC) applications. The incorporation of sulfonic acid groups enables efficient proton transport through well-defined hydrophilic domains, while the aromatic polymer backbone provides mechanical strength and thermal stability. Beyond conventional perfluorosulfonic membranes, sulfonated hydrocarbon polymers such as sulfonated poly (ether ether ketone) and sulfonated polysulfonesss offer adjustable physicochemical properties through controlled functionalization and composite design. The degree of sulfonation was optimized to balance proton transport and dimensional stability. This overview highlights the structure–property–performance relationships of sulfonated PEMs, their electrochemical behaviour in fuel cells, and ongoing strategies to improve conductivity, durability, and long-term stability. Sulfonated polymers continue to represent a versatile and competitive platform for advancing next-generation fuel cell systems.

Keywords: Fuel Cell, PEMs, Sulfonated Polymers,

| PP-57 |

Design of Quinoline-Amide Conjugates Targeting HPV-mediated Proteins to Suppress Cervical Cancer

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Abstract

Cervical cancer remains a major global health burden, with GLOBOCAN 2025 reporting approximately 1.57 million new cases worldwide. Persistent infection with high-risk human papillomavirus 16/18 accounts for more than 70% of cases, and despite advances in vaccination and screening, incidence and mortality remain disproportionately high in low-resource regions. In the search for more effective therapeutics, quinolones—an important class of nitrogen-containing heterocycles—have gained prominence due to their structural versatility, electronic adaptability, and proven activity across diverse pharmacological domains. The quinolone core, originally developed from nalidixic acid and later optimised in fluoroquinolone generations, offers a privileged scaffold capable of modulating key molecular pathways involved in carcinogenesis. Recent investigations have highlighted the potential of quinolone derivatives to target cervical cancer through multiple mechanisms, including DNA intercalation, inhibition of topoisomerase II, induction of oxidative DNA damage, G2/M cell cycle arrest, and restoration of p53-regulated apoptosis. Additionally, metal–quinolone complexes have demonstrated enhanced redox activity and selective cytotoxicity against cervical cancer cell lines. Preclinical studies further reveal significant antiproliferative effects against HeLa and SiHa cells, supported by downregulation of angiogenic and metastatic markers, as well as a strong binding affinity in molecular docking analyses toward HPV oncoproteins. Collectively, these findings position quinolone-based derivatives as promising candidates for developing next-generation therapeutics targeting cervical cancer.

Keywords: Quinolone derivatives, Cervical cancer, HPV-associated proteins, Drug discovery, Antiproliferative activity, Topoisomerase II inhibition, DNA intercalation, Molecular docking, HeLa and SiHa cells.

| PP-58 |

Multicomponent Synthesis and Structure of Novel Spiroindanedione-pyrroloisoquinolines by 1,3-dipolar Cycloaddition of Azomethine Ylide

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Abstract

A series of spiroindanedione-pyrroloisoquinoline derivatives were synthesized through a multicomponent approach using a catalyst-free 1,3-dipolar cycloaddition reaction. In this method, azomethine ylide reacted with novel dipolarophiles, namely (E)-3-aryl-1-(thiophen-2-yl)-prop-2-en-1-ones. The azomethine ylide was generated in situ from ninhydrin and 1,2,3,4-tetrahydroisoquinoline via a [1,5]-prototropic shift pathway. This reaction successfully produced spiroindanedione-pyrroloisoquinoline derivatives as the final products. The developed protocol provides a simple, efficient, and high-yielding route to synthetically useful and biologically important spiroindanedione-pyrroloisoquinoline compounds, with excellent regioselectivity and stereo selectivity. The regiochemistry and molecular structures of the obtained cycloadducts were confirmed using FT-IR, ¹H NMR, ¹³C NMR, and 2D NMR spectroscopic techniques, along with X-ray crystallographic analysis.

Keywords: Spiroindanedione-pyrroloisoquinoline, [3+2]-Cycloaddition, [1,5]-prototropic shift, NMR, X-ray crystal structure analysis.

| PP-59 |

Multifunctional MWCNT Enriched Nickel Cobalt Sulfides Composites for High-Performance Supercapacitors and Dye-Sensitized Solar Cells

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Abstract

In contrast to bare metal oxides and metal sulfides, transition metal sulfides with carbon hybrids were used as high-capacity electrode materials in energy storage devices because of their superior electrical conductivity and quantity of electroactive sites. Here, the hydrothermal approach is used to rationally create the MWCNT enriched nickel cobalt sulfides (NCS/MWCNT) composite architecture. The resulting NCS/MWCNT composite was employed as a current collector in supercapacitor devices and as a counter electrode in dye-sensitized solar cells (DSSCs) to examine the bi-functional electrochemical behaviour. The structural, morphological, chemical composition of the prepared composites were investigated using XRD, SEM, TEM and XPS studies. Notably, the MWCNT incorporated NCS electrode demonstrated superior conductivity and reduced charge transfer resistance at the electrode/electrolyte interface in comparison to its bare composites. Consequently, the J_{SC} of 9.82 mA/cm^2 , V_{OC} of 0.72 V , fill factor (FF) of 0.68 , and power conversion efficiency of 4.81% were all delivered by the DSSC device constructed with MWCNT integrated NCS. These results are equivalent to those of Pt CE (5.12%). Additionally, MWCNT embedded NCS retains approximately 79.1% of its capacitance over 2000 charging-discharging cycles, with a maximum specific capacity of 361 F/g at a current density of 2 A/g .

Keywords: Energy materials, MWCNT, Nanomaterials, DSSC

| PP-60 |

Cellulose Acetate/SrO Composite Biopolymer Membranes: Structural, Functional and Thermal Analysis

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Abstract

Biopolymer membranes reinforced with inorganic oxides provide an effective strategy to improve structural stability and thermal resistance through simple and scalable fabrication approaches. In this study, strontium oxide (SrO) incorporated cellulose acetate (CA) composite membranes were successfully prepared using a solution casting method. X-ray diffraction (XRD) analysis confirmed the successful integration of crystalline SrO within the CA structure and revealed noticeable modifications in the structural characteristics and crystallinity of the polymer upon oxide incorporation. Fourier transform infrared spectroscopy (FTIR) was employed to examine functional group interactions, indicating effective interfacial interactions between SrO particles and the cellulose acetate chains, supporting composite formation. Field-emission scanning electron microscopy (FESEM) demonstrated distinct variations in surface morphology and oxide distribution within the polymer framework, suggesting that SrO incorporation influences the microstructural organization of the membrane. Thermal stability and degradation behavior were evaluated using thermogravimetric and differential thermal analysis (TGA–DTA), revealing that the presence of SrO alters the decomposition pathway of CA and enhances its resistance to thermal degradation compared to the pristine membrane. Overall, the developed CA/SrO composite membrane exhibits improved structural integrity and thermal performance, indicating its suitability for advanced membrane-based functional and separation-related applications.

Keywords: Biopolymer membrane, Cellulose acetate, Metal oxide, Solution casting method

| PP-61 |

Bimetallic MOF coated screen printed as disposable electrode for electrochemical detection of Paracetamol

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Abstract

The rational integration of bimetal-organic frameworks (MOFs) with distinct structural dimensionalities offers a powerful strategy for constructing advanced hybrid architectures with enhanced physiochemical properties. In this work, CoNi-based bimetallic MOF was successfully synthesized using 2 Methyl Imidazole via facile coprecipitation method. Structural and phase purity of CoNi-MOF were confirmed by X-ray diffraction (XRD) analysis. The CoNi-MOF modified SPE exhibited in 0.1 M PBS (pH 7.2), with anodic and cathodic peak potentials at +0.25 V and -0.10 V (vs. Ag/AgCl), respectively. Under optimized potential of +0.60 V, the sensor achieved an ultralow detection limit (0.09 nM). The enhanced analytical performance is attributed to the synergistic interaction between the Co²⁺/Ni²⁺ bimetallic active sites, further increased electrochemically active surface area, and efficient adsorption of paracetamol molecules. The sensor further demonstrated excellent selectivity, repeatability, and operational stability, highlighting the broader applicability of this hybrid design for advanced electrochemical and electrocatalytic systems.

Keywords: Bimetallic CoNi-MOF; Electrochemical sensing; Paracetamol detection.

| PP-62 |

Limit to DNA Reactive Substances in Drug Substances and in Drug Products

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Abstract

DNA-reactive substances can directly damage DNA even at very low exposure levels, leading to mutations and potentially causing cancer, and these mutagenic carcinogens are typically identified using the bacterial reverse mutation (Ames) assay, which serves as the primary method for detecting mutagenicity. In contrast, other genotoxic agents that act through non-mutagenic mechanisms generally exhibit threshold effects and do not pose carcinogenic risk at the impurity levels normally encountered in pharmaceutical products. Therefore, evaluating potentially mutagenic impurities through bacterial mutagenicity testing is essential to determine risk and establish necessary controls. Structure-based assessments further support prediction of mutagenic potential by incorporating known toxicological data, published literature, and computational toxicology tools. To aid regulatory decision-making, the Threshold of Toxicological Concern (TTC) concept was developed to define an intake value for untested chemicals below which the risk of carcinogenic or other toxic effects is negligible. The TTC approach is intentionally conservative, relying on linear extrapolation from tumor-inducing doses (TD50) to a theoretical 1 in 10⁶ cancer risk, using data from the most sensitive species and tumor sites. For mutagenic impurities in drug substances and products, an acceptable intake of 1.5 µg/day is generally justified, corresponding to a theoretical 10⁻⁵ excess lifetime cancer risk. However, certain structural classes are so highly potent that even exposures below the TTC may present concern; this “cohort of concern” includes aflatoxin-like compounds, N-nitroso compounds, and alkyl-azoxy compounds.

Keywords: Genotoxic, Mutagenicity, Toxicological Concern and cohort of concern

| PP-63 |

One-pot Multicomponent Synthesis of Bioactive Dispiro-indenoquinoline Pyrrolidine Derivatives

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Abstract

A chemo-, regio- and stereoselective synthesis of hitherto unexplored novel class of dispiropyrrrolidine embedded with indenoquinoline hybrid heterocycle has been achieved employing an eco-friendly multicomponent 1,3-dipolar cycloaddition cascade protocol. The dipolarophile, 2,6-di(arylmethylidene)-4-methylcyclohexanone reacts with non-stabilized 1,3-dipole component derived from indenoquinolinone and sarcosine through decarboxylative cascade reaction pathway affording dispiropyrrrolidine embedded with indenoquinoline as the final product. The structure of dispiropyrrrolidine embedded with indenoquinoline was confirmed through IR, ¹H NMR and ¹³C NMR analyses. Further, stereochemistry of the dispiropyrrrolidine compound was undoubtedly determined through single crystal XRD analysis

Keywords: Dispiropyrrrolidine, Indenoquinoline, 1,3-Dipolar cycloaddition, X-Ray diffraction analysis

| PP-64 |

Process Development of (2S,3R)-1-(Dimethylamino)-3-(3-Methoxy phenyl)-2-Methyl Pentan-3-OL

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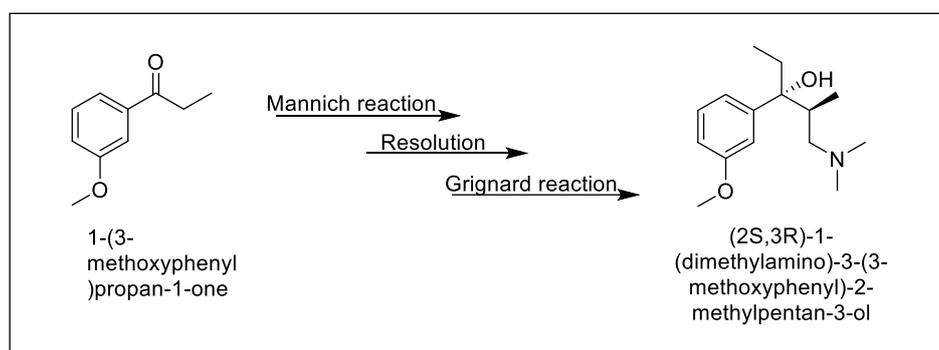
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Abstract

Tapentadol is sold under the brand name of Nucynta and Nucynta ER (extended release) among others, is a medication used in the treatment of moderate to severe Pain. (2S,3R)-1- (dimethylamino)-3-(3-methoxyphenyl)-2-methyl pentane-3-ol is one of the key intermediates of Tapentadol. It is commercially available intermediate in the global market and widely used in the synthesis of Tapentadol. The (2S,3R)-1- (dimethylamino)-3-(3-methoxyphenyl)-2-methyl pentan-3-ol. It is the very small and two chiral centered molecule but it has the several chemical modifications included like Mannich reaction, resolution, Grignard reaction, as per our route of synthesis some of those reaction simplified for control the number of crystallization, filtration, usage of number of solvents, time cycles, followed by control the cost of manufacturing and to increase the productivity in commercial scale. The structure of Tapentadol has been elucidated by elemental analysis (C, H, N and O), Spectroscopic analyses (IR, ¹H-NMR, ¹³C-NMR,) and mass spectrometry. All data are consistent with the proposed structure.

Keywords: Methoxy propiophenone, DBTA, Acetone, Paraformaldehyde, Dimethylamine hydrochlorid



| PP-65 |

Dual-mode Schiff Base Chemosensor for Selective Detection of Cu²⁺ and Zn²⁺ in DMSO: Mechanism and Practical Applications

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Abstract

The development of single-component chemosensors for multianalyte detection is challenging yet highly desirable. We presented a novel Schiff-base fluorescent chemosensor 3-(2-((2-hydroxynaphthalen-1-yl) methylene) hydrazinyl) quinoxalin-2(1H)-one (HNQH) that achieved solvent-dependent discrimination of metal ions via distinct fluorescence and Calorimetric pathways. In DMSO, HNQH selectively recognized Zn²⁺ via 1:1 chelation-enhanced fluorescence (CHEF) mechanism with green emission and HNQH exhibits selective colorimetric chemosensor properties for Cu²⁺ ions. Job's plot, FT-IR, NMR titration, and DFT calculations verified the coordination structures and correlated the spectral differences with the distinct metal-binding affinities. HNQH achieved nanomolar detection limits, excellent selectivity, and anti-interference capability, with practical applicability confirmed through environmental water analysis and paper-based test strips. This work provides a versatile sensing strategy and structural insights for designing multi-responsive chemosensors based on coordination-controlled emission.

Keywords: Schiff's base, Multi-analyte Chemosensor, Metal ion recognition, DFT, Practical utility.

| PP-66 |

Photocatalytic Degradation of Oxytetracycline Using Co-Cu Co-doped $\text{Al}_2\text{O}_3@Fe_2\text{O}_3$ Nanocomposites

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Abstract

Antibiotics containing wastewater from pharmaceutical industries have become a harmful organic pollutant and needs to be seriously treated, and one of the important antibiotics is oxy tetracycline. In this study, we synthesized a visible light active Co-Cu co-doped $\text{Al}_2\text{O}_3@Fe_2\text{O}_3$ nanocomposite by the co-precipitation method and employed as a photocatalyst for the degradation of oxytetracycline. The obtained nanocomposite was characterized using UV-DRS, FT-IR, XRD, XPS, and FeSEM. The UV-DRS displayed optical information with strong absorption peaks at 226 nm and 270 nm of Al and Fe, and a band gap energy of 2.0 eV. FT-IR spectroscopy shows a band at 620 cm^{-1} which is attributed to metal oxide vibrational stretching. XRD analysis showed a rhombohedral crystal structure the nanocomposite. The photocatalytic activity of the prepared sample was investigated by removal of oxytetracycline in contaminated water under sunlight. The photodegradation analysis indicated about 70% of the degradation occurred within 90 minutes. The result indicates the Co-Cu co-doped $\text{Al}_2\text{O}_3@Fe_2\text{O}_3$ nanocomposite is an efficient, eco-friendly, and economical photocatalyst for the removal of persistent pharmaceutical pollutants from water.

Keywords: Co–Cu co-doped $\text{Al}_2\text{O}_3@Fe_2\text{O}_3$ nanocomposite, Oxytetracycline, Photo degradation, Co-precipitation, Wastewater treatment.

| PP-67 |

A Dual-channel Chemosensor Based on Carbazole Based Schiff Base for Fluorescence Detection and Colorimetric Recognition of Glutamic Acid

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Abstract

A colorimetric and fluorescent dual-channel glutamic acid (Glu) chemosensor (*Z*) (((9ethyl 9H-carbazole3yl)imino)methyl)naphthalen-2-ol (9EACHN) bearing an aldehyde group has been designed and synthesized. This structurally simple chemosensor displays rapid response and high selectivity for Glu over other common amino acids in ACN/H₂O (9: 1, v/v, buffered by 10mM PBS buffer at pH = 7.2) solution. The chemosensor interacted with Glu to form intermolecular hydrogen bonds with significantly quenched fluorescence, switching from weak green fluorescence to no fluorescence. Moreover, 9EACHN can also successfully detect glutamic acid by absorption spectroscopy, which exhibited an UV–vis spectrum change, while its color changed from colorless to turbid white under natural light. Job's plot indicates that the binding stoichiometry between the chemosensor 9EACHN and the targeted amino acid Glu is 1:1. Hence, our experimental findings and theoretical findings very strongly suggest that 9EACHN can be used as chemosensor for detecting Glu in future.

Keywords: Colorimetric detection of glutamic acid, Carbazole, DFT.

| PP-68 |

DIELECTRIC AND MORPHOLOGICAL ANALYSIS POLY (m-PHENYLENEDIAMINE)/ $\text{CoMnFe}_2\text{O}_4$ NANOCOMPOSITES

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Abstract

Polymer/ $\text{CoMnFe}_2\text{O}_4$ spinel ferrite nanoparticles were successfully synthesized using the sol-gel auto-combustion method, which is a simple, cost-effective, and efficient route for producing homogeneous nanostructured materials. To dispersed nanocomposite material into polymer via poly (m- phenylenediamine). The prepared polymer material was systematically characterised to investigate their crystal structure, morphology, elemental composition, and magnetic behaviour using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and field-emission scanning electron microscopy (FESEM). XRD analysis confirmed that the synthesised samples exhibit a single-phase cubic spinel structure without secondary impurity phases, indicating the successful formation of cobalt-doped manganese ferrite. The average crystallite size was calculated from the diffraction peaks, revealing nanoscale dimensions, while lattice strain present in the samples was evaluated, suggesting slight structural distortion due to cobalt and manganese substitution. These structural modifications play a significant role in tailoring the functional properties of the material. FTIR spectra exhibited characteristic absorption bands corresponding to metal–oxygen stretching vibrations in the tetrahedral and octahedral sites of the spinel lattice, confirming the formation of Co-O, Mn-O, and Fe-O bonds. FESEM images revealed that the polymer-dispersed $\text{CoMnFe}_2\text{O}_4$ ferrite nanoparticles are predominantly spherical in shape with relatively uniform grain distribution and reduced agglomeration. The polymer matrix effectively prevents excessive particle clustering, which is beneficial for enhancing surface area and interfacial properties. The substitution of cobalt magnetic ions with Mn^{2+} ions enables effective tuning of magnetic characteristics by modifying cation distribution and superexchange interactions within the spinel structure. This tunability, combined with good dielectric behaviour and structural stability, makes polymer/ $\text{CoMnFe}_2\text{O}_4$ ferrite nanocomposites promising candidates for dielectric materials in supercapacitor applications, where efficient energy storage, high stability, and multifunctional performance are essential.

Keywords: $\text{CoMnFe}_2\text{O}_4$; Ferrite; XRD; FESEM; XPS and supercapacitor.

| PP-69 |

Investigation on Cu-doped BiLaO₃ Nanoparticle as a Potential Effluent Treatment of Photocatalysis Dye Degradation

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Abstract

Photocatalytic degradation is considered an effective strategy for removing hazardous dye contaminants from wastewater. In this study, pure BiLaO₃ and Cu-doped BiLaO₃ nanoparticles were synthesized via a hydrothermal method and evaluated for the degradation of malachite green (MG) under visible light irradiation. XRD analysis revealed slight lattice distortion upon Cu doping, indicating structural modification without secondary phase formation. The reduced band gap energy and improved charge separation efficiency significantly enhanced photocatalytic performance. The optimally doped Cu–BiLaO₃ sample achieved markedly higher MG dye degradation efficiency compared to pristine BiLaO₃, demonstrating accelerated reaction kinetics under visible light. The enhanced activity is attributed to improved electron–hole separation, increased reactive oxygen species generation, and greater surface area. This study highlights Cu-doped BiLaO₃ as an efficient photocatalyst for treating dye-contaminated wastewater and environmental remediation applications.

Keywords: Cu-doped BiLaO₃, Hydrothermal synthesis, Photocatalysis, Malachite Green, Visible Light

| PP-70 |

A Highly Selective Ratiometric and Colorimetric Detection of Ni²⁺ and Co²⁺ ions using Schiff Base Ligand

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Abstract

The efficacy of superficial molecular receptors for spectroscopic and colorimetric detection of metal ions is crucial for environmental and biological importance. Herein, the new **chemosensor (ANES)** acts as a chemosensor for the selective detection of Ni²⁺ and Co²⁺ ions. The chemosensor selective detection behavior for Ni²⁺ and Co²⁺ ion is observed by the change in color (colorless to yellow), redshifts in UV-visible spectra, and ratiometric enhancement in fluorescence probes studies. In addition, the colorimetric analyses are observed under visible and UV light show interesting colorimetric changes due to the d-d transitions. The quantitative parameters of chemosensor are determined as the limit of detection (LOD) and limit of quantitation. To evaluate the mechanistic pathway of probe and metal by theoretical insights and the probe shows good ability to detect the Ni²⁺ and Co²⁺ ions in the environmental samples with good recovery percentage.

Keywords: Colorimetric detection for Ni²⁺ and Co²⁺ ions, DFT, Environmental water and soil samples.

| PP-71 |

Synthesis of Polymer/ZnNiFe₂O₄ Nanocomposites for Dielectric Applications

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Abstract

A series of poly(*m*-phenylenediamine)/zinc nickel ferrite (PmPD/ZnNiFe₂O₄) nanocomposites with varying ferrite loadings were successfully synthesized via an in situ oxidative polymerization method. The incorporation of ZnNiFe₂O₄ nanoparticles into the PmPD matrix was achieved through uniform dispersion during polymer growth, enabling strong interfacial interaction between the organic polymer backbone and inorganic ferrite phase. The structural, thermal, morphological, and dielectric properties of the prepared nanocomposites were systematically investigated using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), and thermogravimetric analysis (TGA). XRD patterns confirmed the presence of crystalline spinel ZnNiFe₂O₄ within the amorphous PmPD matrix, while FTIR spectra verified the successful formation of the polymer and its interaction with ferrite nanoparticles. TEM analysis revealed well-dispersed ZnNiFe₂O₄ nanoparticles anchored onto the polymer matrix, leading to modification of the intrinsic spherical morphology of PmPD. The nanocomposites exhibited enhanced thermal stability compared to pristine polymer, with thermal resistance increasing proportionally to ferrite content, indicating improved structural integrity due to polymer–ferrite interactions. Dielectric studies demonstrated that the dielectric constant and AC conductivity strongly depend on applied frequency, temperature, and nanoparticle concentration. The dielectric constant decreased with increasing frequency due to interfacial polarization effects, while AC conductivity increased with temperature, confirming semiconducting behaviour. Enhanced dielectric performance at higher ferrite loadings suggests potential applicability in energy storage devices, electromagnetic interference shielding, and high-performance dielectric capacitors. Overall, the synthesized PmPD/ZnNiFe₂O₄ nanocomposites exhibit tunable structural and electrical properties, making them promising candidates for advanced electronic and electrochemical applications.

Keywords: ZnNiFe₂O₄, Ferrite, Sol-gel process, XRD, FESEM, FTIR, XPS analysis, Dielectric properties and supercapacitor.

| PP-72 |

Luminescence sensing, DFT, Extraction and Monitoring of Cr³⁺ and Al³⁺ Via the Application of First Derivative Fluorescence Spectroscopy

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Abstract

A novel pyridine core containing Schiff base (HNAHP) has been developed as a turn-on chromofluorogenic sensor for chromium (III) (Cr³⁺) and aluminium (III) (Al³⁺) ions in an aqueous environment. It has been characterized by absorption, emission, FTIR, NMR and mass studies. The receptor shows a significant colour change from blue to green under UV light, in the presence of Al³⁺ and Cr³⁺ with limit of detection (LOD) and association constant (K_{ass}) were performed. In the presence of monovalent and divalent ions (Na⁺, Hg²⁺, Pb²⁺, Cd²⁺, Ni²⁺, Co²⁺, Cu²⁺, Fe²⁺, Mn²⁺ and Zn²⁺), no significant changes are observed in their spectral patterns. Upon excitation, the ligand exhibits a turn-on emission in the presence of Al³⁺ and Cr³⁺, which may be due to chelation-enhanced fluorescence (CHEF), which is further supported by DFT/TDDFT studies. Herein, Al³⁺, Cr³⁺ and EDTA have been used to design an advanced level combinational INHIBIT gate. Moreover, this ligand is capable of selectively extracting Al³⁺ and Cr³⁺ from an aqueous mixture of other metal ions by the liquid-liquid extraction method. In order to estimate Al³⁺ and Cr³⁺ concentrations simultaneously in the mixture without prior separation, first derivative normal fluorescence spectroscopy has been applied.

Keywords: Fluorescence turn on for Al³⁺ and Cr³⁺ ions, DFT/TDFT, Liquid-liquid extraction.

| PP-73 |

Fe₂O₃/BaSO₄ Nanocomposite: Preparation, Characterization and Pigment Property

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Abstract

Iron (III) oxide (Fe₂O₃)-based composites have much attention in various fields including catalysis, pigment and biomedical applications. Especially, Fe₂O₃-based composites have been reported for their pigment features. In this context, we have prepared Fe₂O₃/barium sulphate (BaSO₄) composite by a two-step process. First, FeOOH has been prepared by hydrolysis of method along with precipitation of BaSO₄. In the second step, the as-prepared FeOOH/BaSO₄ composite was converted into Fe₂O₃/BaSO₄ composite by a thermal decomposition method. The calcination temperature of FeOOH/BaSO₄ was fixed as 600 °C for 4 h. The as-prepared Fe₂O₃/BaSO₄ composite were examined by X-ray diffraction (XRD), Fourier transform infrared (FTIR), and UV-visible spectroscopic techniques. The formation of crystalline Fe₂O₃ and BaSO₄ was confirmed by XRD. The presence of functional groups including Fe-O, Ba-O and S-O stretching vibrations were confirmed by observing characteristic FTIR bands. The d-d transition and ligand to metal charge transfer transitions were also noted in the UV-Visible spectrum of Fe₂O₃/BaSO₄ composite. The chromaticity features of Fe₂O₃/BaSO₄ composite were analysed by the CIE 1931 method (UV-visible spectrophotometer). The CIE x and CIE y coordinates were determined. The ink application of as-prepared Fe₂O₃/BaSO₄ composite has also been tested.

Keywords: Fe₂O₃, BaSO₄, Hydrolysis, Thermal decomposition route, Pigments,

| PP-74 |

Thermal and Morphology Analysis of Poly(*m*-phenylenediamine) /NiMnFe₂O₄ Nanocomposite

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Abstract

Poly(*m*-phenylenediamine) (PmPD)/NiMnFe₂O₄ nanocomposites were synthesized by an in situ oxidative polymerization method using two different weight percentages (10% and 20%) of NiMnFe₂O₄ nanoparticles. Structural analysis through X-ray diffraction (XRD) confirmed the successful incorporation of spinel ferrite nanoparticles into the PmPD matrix. Scanning electron microscopy (SEM) showed sphere-like morphology for pure PmPD, while nanocomposites exhibited modified surface features due to nanoparticle dispersion. Dielectric studies carried out over varying frequencies and temperatures revealed that the dielectric constant decreases with increasing frequency and increases with higher ferrite content, indicating enhanced interfacial polarization. Magnetic measurements at room temperature confirmed ferromagnetic behaviour of both NiMnFe₂O₄ nanoparticles and the prepared nanocomposites, with magnetization increasing as ferrite concentration increased. Thermogravimetric analysis (TGA) demonstrated improved thermal stability of the nanocomposites compared to pure PmPD. These results suggest potential applications in multifunctional electronic and magnetic devices.

Keywords: Poly(*m*-phenylenediamine) (PmPD), NiMnFe₂O₄, Dielectric properties, Magnetic nanocomposites

| PP-75 |

Photocatalytic Degradation of Antibiotics using Zn–Fe Doped CuO Nanoparticles

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Abstract

The heavy usage of antibiotics now causes release of antibiotic contaminants into water sources as a phenomenon has been a critical environmental issue as a result of their persistence and adverse impacts. This paper presents the synthesis of Zn-Fe doped CuO nanoparticles that are prepared by a simple and cheaper co-precipitation technique and characterized in terms of their photocatalytic activity in the degradation of norfloxacin pollutants. The nanoparticles were prepared and the optical properties, functional groups and crystal structure of the prepared nanoparticles were studied using UV-Visible spectroscopy, FTIR and X-ray diffraction (XRD) methods. The UV- Vis spectrum showed that there was intense absorption at the UV portion with clear visibility of light to 800nm, which is the charge transfer transitions and d-d transitions at CuO which proves that CuO is really a semiconductor. The FTIR analysis revealed a typical Cu-O stretching vibrations, which proved the presence of a monoclinic CuO. XRD patterns had clearly visible diffraction peaks confirming the purity of the phases and the nanocrystalline structure. The photodegradation studies reveal that Zn-Fe doped CuO nanoparticles have a good photocatalytic activity and would be useful in the degradation of norfloxacin pollutants in wastewater under light irradiation. The photodegradation was about 70% degradation in 60 minutes. The result indicates the Zn-Fe doped CuO nanocomposite is an efficient, eco-friendly, and economical photocatalyst for the removal of persistent pharmaceutical pollutants from water. This paper has characterized the prospect of doped CuO nanomaterials as effective and clean photocatalysts in the treatment of water.

Keywords: The Zn-Fe doped CuO nanocomposite, Norfloxacin, Photocatalytic degradation, Co-precipitation method, Antibiotic wastewater treatment

| PP-76 |

The Effect of Carbon Doped Magnesium Oxide with Thorium Electro-catalyst in the Aluminium Air Battery

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Abstract

The development of a rechargeable aluminium-air battery with a large capacity and extended durability in charge-discharge electrochemical processes was the aim of this work. The main challenges keeping Al-air batteries becoming widely commercialized is the development of extremely effective, affordable, and long-lasting electro catalysts for the oxygen reduction reaction. In this work, four common kinds of carbon black are used along with a rare earth salt namely thorium nitrate and MgO. The exceptional qualities of aluminium air batteries include their low cost, excellent recyclability, low weight, high energy density, and environmental friendliness. The great energy density and low cost of aluminium air batteries make them a promising source of electronic power. Aluminium exhibits great potential as an energy carrier because to its abundant supply, low cost, high capacity and energy density, and environmental friendliness. The features of air batteries are studied electro-modelling with the goal of using aluminium-air batteries as an alternative energy storage method in the future.

Keywords: Thorium Nitrate, Magnesium Oxide, Carbon, Aluminium Air battery

| PP-77 |

The Effect of the Coconut Coir Carbon doped Zirconium Oxychloride Octahydrate with Epoxy Resin as Cathode Material in Aluminium Air Battery

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Abstract

The present invention is to provide an air cathode for aluminium air battery, having excellent discharge performance and an aluminium air battery. Disclosed is an air cathode for aluminium air battery, using oxygen as an active material and configured to form an air battery comprising the air cathode, an aluminium anode and a separator layer along with an electrolyte present between the air cathode and the aluminium anode, the air cathode comprising: an Zirconium Oxychloride Octahydrate as the electrode catalyst, which is active against at least oxygen reduction reaction; at least one carbon as conductive material and an organic binder Epoxy Resin(Polyepoxides).

Keywords: Zirconium Oxchloride, Epoxy Resin, Coconut Coir Carbon, Aluminium air battery

| PP-78 |

Photocatalytic Properties of Fe₂O₃/g-C₃N₄ Composite

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Abstract

Herein, iron (III) oxide (Fe₂O₃)/graphitic carbon nitride (g-C₃N₄) composite was prepared to explore its photocatalytic application in dye treatment. By using hydrolysis method, FeOOH was prepared in presence of g-C₃N₄ and the resultant mixture was thermally converted into Fe₂O₃/g-C₃N₄. The g-C₃N₄ powder was synthesised by thermal polymerisation of melamine at 450 °C. The formation of Fe₂O₃ crystals and g-C₃N₄ were confirmed by powder X-ray diffraction analysis. The presence of Fe-O (metal - oxygen) and C-N bonds in Fe₂O₃/g-C₃N₄ composite was determined by Fourier transform (FTIR) infrared spectroscopy. Fe₂O₃/g-C₃N₄ composite shows good absorption in the visible light region. Tauc plot was employed to calculate the band gap of Fe₂O₃/g-C₃N₄ composite. The photocatalytic properties of Fe₂O₃/g-C₃N₄ composite were examined by using hydrogen peroxide (H₂O₂)-mediated degradation of methylene blue (1×10⁻⁵ M, 100 ml) and Congo red (3×10⁻⁵ M, 100 ml) in water medium under visible light irradiation. For comparison, the photocatalytic experiments have also been conducted in the absence of H₂O₂. Fe₂O₃/g-C₃N₄ composite showed photocatalytic activity under the optimized experimental condition and it is expected to become a great catalyst in the photocatalytic treatment of dye effluents.

Keywords: Fe₂O₃/g-C₃N₄, Composite, Photocatalysis, H₂O₂, Methylene blue, Congo red.

| PP-79 |

Evaluation of NIR Reflective Property of BiVO₄/BaSO₄ Composites

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Abstract

In this paper, bismuth vanadate (BiVO₄)/barium sulphate (BaSO₄) composites were prepared to find their NIR reflective pigment features. First, BiVO₄ pigment powder was prepared by using thermal decomposition method. Subsequently, BaSO₄ was precipitated in presence of as-prepared BiVO₄ powder. The content of BaSO₄ with respect to BiVO₄ is varied from 10 to 50%. The as-prepared BiVO₄/BaSO₄ composite were examined by X-ray diffraction (XRD), Fourier transform infrared (FT-IR), and UV-visible spectroscopic techniques. The formation of crystalline BiVO₄ and BaSO₄ was confirmed by XRD. The presence of functional groups including Bi-O, V-O, Ba-O and S-O stretching vibrations were confirmed by observing characteristic FTIR bands. The d-d transition and ligand to metal charge transfer transitions were also noted in the UV-Visible spectrum of BiVO₄/BaSO₄ composite. The chromaticity features of BiVO₄/BaSO₄ composite were analysed by the CIE 1931 method (UV-visible spectrophotometer). The CIE x and CIE y coordinates were determined. The ink application of as-prepared BiVO₄/BaSO₄ composite has also been tested. Additionally, NIR reflective property of BiVO₄/BaSO₄ composites has also been evaluated.

Keywords: BiVO₄, BaSO₄, Thermal decomposition, Precipitation, Pigment.

| PP-80 |

Benzothiazole-Lepidine based fluorescent Probe for the Selective Detection of Cyanide in Solution

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Abstract

In this work, benzothiazole–lepidine based fluorescent probe (ALE) was successfully designed and synthesized for the selective detection of cyanide ions in solution. Cyanide is a highly toxic and environmentally hazardous species, and its rapid and reliable detection is of great importance in environmental monitoring and industrial safety. With this motivation, a structurally conjugated fluorescent probe was developed through a straightforward multi-step synthetic procedure. The synthesis began with the formation of 2-(benzo[d]thiazol-2-yl) phenol (ASE) from 2-aminothiophenol and salicylaldehyde. This intermediate was further functionalized to obtain the aldehyde derivative (AHT), which was subsequently condensed with a lepidine derivative to yield the final probe molecule, ALE. The synthesized compound was thoroughly characterized using FT-IR, ¹H NMR, ¹³C NMR, and ESI-MS techniques, confirming the successful formation of the desired molecular structure. The optical sensing properties of ALE were investigated using UV-Visible absorption and photoluminescence spectroscopy. Upon gradual addition of cyanide ions, significant changes were observed in both absorption and emission spectra, indicating strong interaction between the probe and cyanide. The sensing mechanism is proposed to involve a nucleophilic attack of cyanide on the electron-deficient styryl unit of ALE. This reaction disrupts the extended π -conjugation and inhibits the intramolecular charge transfer (ICT) process, leading to a measurable and distinct optical response. Importantly, the probe exhibited high sensitivity, rapid response time, and excellent selectivity toward cyanide in the presence of other competing ions. These findings demonstrate that ALE is a promising and efficient fluorescent chemo-sensor with potential applications in environmental analysis and safety monitoring.

Keywords: Benzothiazole, Fluorescent probe, Cyanide ions detection, Intramolecular charge transfer (ICT), Optical sensing.

| PP-81 |

Recent Trends in Various Carbon Film/Materials and Cell Design for Aluminium Ion Battery

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Abstract

Aluminium-ion batteries are increasing interest as alternatives to lithium-ion batteries, as they use more abundant materials and suffer from fewer safety risks. Recent years have seen a notable improvement in aluminium-ion battery performance across all criteria pertinent to batteries, making them a viable substitute. The main challenges keeping Al-air batteries becoming widely commercialized is the development of extremely effective, affordable, and long-lasting electro catalysts for the oxygen reduction reaction. This work compares three common forms of carbon: carbon N330, carbon KS44, carbon N550 felt as aluminium-ion cathodes. Al-based batteries are currently being considered as potential energy storage technologies. The features of ion batteries are studied electro- modelling with the goal of using aluminium-ion batteries as an alternative energy storage method in the future.

Keywords: Carbon N330, Carbon KS44, Carbon N550, Magnesium oxide, Polyvinyl alcohol.

| PP-82 |

Amine Functionalization of Biochar for Tailoring Surface Charge and Enhancing Zero-point Charge (pHzpc)

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Abstract

Surface charge is a key factor influencing the adsorption performance of biochar toward anionic contaminants. In this study, NaOH-activated biochar derived from lotus seed pericarp was modified through NH₄OH-assisted amine functionalization to enhance its point of zero charge (pHzpc). Sonication-assisted functionalization was optimized using a full factorial design (FFD) by systematically evaluating the effects of NH₄OH concentration, sonication temperature, and time. Statistical analysis revealed that NH₄OH concentration had a significant effect on pHzpc, while sonication temperature and time showed no significant independent effects but exhibited strong interaction effects with NH₄OH concentration. Response surface optimization identified the optimal conditions as 25 % NH₄OH concentration, 50 °C sonication temperature, and 2 h sonication time, yielding a maximum predicted pHzpc of 6.86. FTIR analysis confirmed successful amine functionalization through the appearance and enhancement of nitrogen-containing functional groups. These results demonstrate that controlled NH₄OH-assisted sonication is an effective approach for tailoring biochar surface charge, enhancing its suitability for anionic contaminant removal

Keywords: Biochar functionalization, Amine modification, Point of zero charge, Surface charge tailoring

| PP-83 |

Benzothiazole-based Fluorescent Receptor for the Selective Detection of Phosgene in Solution

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Abstract

The detection of highly toxic industrial chemicals is of paramount importance for environmental safety and human health. Among these chemicals, phosgene is a potent carbonylating agent widely used in organic synthesis and large-scale industrial applications, yet it poses severe health hazards even at low concentrations. In this study, a benzothiazole-based fluorescent chemosensor (ABDE) was designed and synthesized for the selective and sensitive detection of phosgene in solution. The receptor was synthesized through a multi-step reaction sequence involving condensation, Vilsmeier-Haack formylation, quaternization, and final coupling reactions, followed by purification and structural characterization using FT-IR and ¹H-NMR spectroscopy. The sensing performance of the synthesized probe was evaluated using UV-Visible absorption and fluorescence spectroscopy. Upon interaction with phosgene, the receptor exhibited a significant fluorescence response attributed to a specific chemical reaction that alters the electronic structure of the benzothiazole fluorophore. The probe demonstrated high selectivity, rapid response, and sensitivity toward phosgene compared to other potential interfering species. Density Functional Theory (DFT) studies further supported the proposed sensing mechanism. This work highlights the potential of benzothiazole-based fluorescent receptors as efficient tools for real-time monitoring of phosgene in environmental and laboratory settings.

Keywords: Benzothiazole derivative, Fluorescent probe, Phosgene detection, Intramolecular charge transfer (ICT), Optical sensing.

| PP-84 |

Synthesis and Characterization of Poly(m-phenylenediamine)/ZnMnFe₂O₄ Nanocomposites

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Abstract

ZnMnFe₂O₄ nanoparticles were synthesised using the auto-combustion method. A series of poly(m-phenylenediamine)/ZnMnFe₂O₄ nanocomposites containing various concentrations of ZnMnFe₂O₄ were prepared by the in situ oxidative polymerisation method. The composites were characterised using standard techniques such as XRD, FTIR, FESEM, and TGA, along with dielectric property analysis. The structural properties of poly(m-phenylenediamine)/ZnMnFe₂O₄ nanocomposites were investigated. FESEM results showed good dispersion of ZnMnFe₂O₄ nanoparticles within the polymer matrix. The changes in structural parameters were correlated with morphology and elemental composition obtained from FESEM analysis. Furthermore, the electrochemical performance demonstrated enhanced capacitive properties, including high specific capacitance, good rate performance, and excellent cycling durability. The results of poly(m-phenylenediamine)/ZnMnFe₂O₄ nanocomposites indicate that it has strong potential for advanced dielectric energy storage and supercapacitor applications.

Keywords: ZnMnFe₂O₄, Poly(m-phenylenediamine), Auto-combustion, Energy storage, and Supercapacitor.

| PP-85 |

A Triphenylamine based Probe for the Ratiometric Detection of Phosgene in Solution

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Abstract

Phosgene (COCl₂) is a highly toxic industrial chemical widely used in the synthesis of polycarbonates, isocyanates, agrochemicals, and pharmaceuticals. Despite its industrial significance, accidental exposure to phosgene poses severe health risks, including pulmonary oedema and respiratory failure, necessitating the development of rapid and sensitive detection methods. In this study, we report the design and synthesis of a triphenylamine-based fluorescent probe for the Ratiometric detection of phosgene in solution. The probe was constructed by integrating a triphenylamine (TPA) moiety as an electron-donating fluorophore with a reactive recognition site that selectively interacts with phosgene. The sensing mechanism relies on a specific nucleophilic substitution reaction between the probe and phosgene. This structural transformation significantly alters the intramolecular charge transfer (ICT) process of the triphenylamine scaffold, resulting in a distinct ratiometric fluorescence response. Upon addition of phosgene, the probe exhibits a pronounced shift in emission wavelength along with a visible colour change, enabling both spectroscopic and visual detection. The developed probe demonstrates high sensitivity detection, with excellent selectivity over structurally related interfering species such as thionyl chloride, phosphorus oxychloride, and other acyl chlorides. UV–visible absorption and fluorescence titration studies confirm the ratiometric behaviour, while ¹H NMR, ¹³C NMR and mass spectrometric analyses support the proposed sensing mechanism. The probe exhibits good stability and reproducibility in organic solvent systems, indicating its practical applicability for real-time monitoring of phosgene in laboratory and industrial environments. The triphenylamine-based fluorescent probe provides a simple, efficient, and reliable platform for the selective detection of phosgene, contributing to improved chemical safety and environmental monitoring.

Keywords: Triphenylamine, Fluorescent probe, Ratiometric detection, Phosgene sensing, Intramolecular charge Transfer, Selectivity detection

| PP-86 |

Chemical Composition of the Essential Oil from *Anisomeles Malabarica*

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Abstract

Anisomeles malabarica, commonly known as the Malabar catmint, is an herbaceous shrub belonging to the family Lamiaceae and has been traditionally utilized in various herbal preparations across different cultures for its purported medicinal properties. The present study investigates the chemical composition of essential oil from *Anisomeles malabarica*. The essential oil was obtained through hydrodistillation (yield 0.01%) and analyzed using GC-MS. The analysis revealed a complex mixture of bioactive compounds with 5.38% of monoterpenes, 42.7 % of sesquiterpenes, 11.10% of triterpenes and fatty acid and their derivatives 40.80%. Of the 17 monoterpenes identified 2,4-Decadienal, 16 sesquiterpenes identified globulol and of the 5 triterpenes identified Triacontane are the major compounds.

Keywords: *Anisomeles malabarica*, Essential oil, Terpenes, GC-MS.

| PP-87 |

Coumarin based Fluorescent Receptor for the Selective Detection of Environmental Hazardous Analytes

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Abstract

A benzo coumarin–pyrazole–quinolinium conjugated fluorescent receptor (OBCLIA) was rationally designed and synthesized via a multi-step heterocyclic transformation strategy. The synthetic route involved initial formation of a benzo coumarin scaffold followed by phenyl hydrazine-mediated cyclization to afford the corresponding pyrazole derivative. Subsequent Vilsmeier–Haack formylation introduced a reactive aldehyde functionality, which was further coupled with a quaternized lepidium salt through a base-catalyzed Knoevenagel condensation to yield the final π -extended conjugated system. The structure of OBCLIA was comprehensively characterized by FT-IR, ¹H NMR, ¹³C NMR, and ESI–MS spectral analyses, confirming the formation of key functional groups including lactone (–O–C=O) and azomethine (–C=N) linkages. The incorporation of electron-donating and electron-accepting moieties within the molecular framework enhances intramolecular charge transfer (ICT), thereby improving its photophysical properties. The designed receptor is anticipated to exhibit high sensitivity and selectivity toward environmentally hazardous analytes through measurable absorbance and fluorescence emission changes. This study provides a promising strategy for the development of efficient coumarin-based fluorescent chemosensors for environmental monitoring applications.

Keywords: Fluorescent chemosensor, Intramolecular charge transfer (ICT) , π -Conjugation.

| PP-88 |

Synthesis of $\text{Mn}_3\text{O}_4@\text{ZnO}$ Nanocomposites Decorated Poly(m-Phenylenediamine) for Photocatalytic Dye Degradation Application

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Abstract

$\text{Mn}_3\text{O}_4@\text{ZnO}$ nanocomposite were synthesized by co-precipitation method. The prepared nanocomposite was dispersed into poly(m-phenylenediamine) through in-situ oxidative polymerization method using ammonium persulphate as oxidizing agent. The $\text{Mn}_3\text{O}_4@\text{ZnO}$ and PmPD/ $\text{Mn}_3\text{O}_4@\text{ZnO}$ were characterized by XRD (X-ray Diffraction), Fourier transformed infrared spectroscopy (FT-IR), UV-DRS spectroscopy, Scanning Electron Microscope (SEM), Transmission Electron Microscopy (TEM) and X-ray Photoelectron Spectroscopy (XPS) studies. The XRD study confirms the formation of $\text{Mn}_3\text{O}_4@\text{ZnO}$ nanocomposites and PmPD/ $\text{Mn}_3\text{O}_4@\text{ZnO}$. FTIR spectra shows metal-oxygen bonding, and UV-Vis DRS studies indicated a narrowed band gap. The SEM images revealed that dispersion of $\text{Mn}_3\text{O}_4@\text{ZnO}$ nanocomposites in poly(m-phenylenediamine). The TEM images of PmPD/ $\text{Mn}_3\text{O}_4@\text{ZnO}$ were indicated the deposition of $\text{Mn}_3\text{O}_4@\text{ZnO}$ nanocomposites on surface of PmPD. The photocatalytic dye degradation of methylene blue under the behavior of PmPD/ $\text{Mn}_3\text{O}_4@\text{ZnO}$ were analyzed. Finally, photocatalytic dye degradation by using PmPD/ $\text{Mn}_3\text{O}_4@\text{ZnO}$ gives 95% of methylene blue, 93% of malachite green, 88% of Congo red where efficiently degradation occur under UV visible light irradiation. The enhanced activity is attributed to effective charge separation and the generation of reactive oxygen species ($\cdot\text{OH}$, $\text{O}_2\cdot^-$), which drive dye mineralization. The PmPD/ $\text{Mn}_3\text{O}_4@\text{ZnO}$ nanocomposite offers a cost-effective, stable, and reusable photocatalyst, with potential applications in wastewater treatment and environmental remediation.

Keywords: Photocatalytic dye degradation, Nanocomposites, PmPD/ $\text{Mn}_3\text{O}_4@\text{ZnO}$

| PP-89 |

Synthesis and Characterization of La-doped MgCo₂O₄ Nanostructures for Supercapacitor Applications

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Abstract

Lanthanum-doped MgCo₂O₄ nanostructures were successfully synthesized via a facile one-step hydrothermal method and directly grown on nickel foam for high-performance supercapacitor applications. Structural analysis confirmed the formation of La-doped MgCo₂O₄. Morphological studies revealed the formation of interconnected nanostructured architectures uniformly distributed over the nickel foam, providing a large electroactive surface area. Electrochemical measurements were conducted to evaluate the specific capacitance, cycling stability, and rate capability of the La-doped MgCo₂O₄ electrodes at various current densities. The performance was compared with pristine MgCo₂O₄ to assess the influence of lanthanum doping on the electrochemical properties. These investigations aim to demonstrate the potential of La-doped MgCo₂O₄ nanostructures as promising electrode materials for next-generation high-performance supercapacitors.

Keywords: La-doped MgCo₂O₄, Hydrothermal synthesis, Spinel nanostructures, Supercapacitor

| PP-90 |

Enhanced Visible-Light Photocatalytic Removal of Antibiotics Using Ag-Doped Rare Earth Cobaltate Nanostructures

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Abstract

The widespread contamination of aquatic environments with antibiotic residues poses a serious environmental threat due to their persistence, bioaccumulation, and contribution to antimicrobial resistance. Conventional wastewater treatment techniques are often inadequate for removing such pharmaceutical pollutants, highlighting the need for advanced remediation approaches. In this study, silver-doped rare earth (RE) cobaltate was synthesized through a co-precipitation method and employed as a visible-light-responsive photocatalyst for antibiotic degradation. RE doping enhanced light absorption, narrowed the bandgap, and improved charge separation efficiency. Characterization results confirmed successful Ag incorporation, which promoted effective reactive oxygen species generation. Conventional wastewater treatment techniques are often inadequate for removing such pharmaceutical pollutants, highlighting the need for advanced remediation approaches. In this study, silver-doped rare earth (RE) cobaltate was synthesized through a co-precipitation method and employed as a visible-light-responsive photocatalyst for antibiotic degradation. RE doping enhanced light absorption, narrowed the bandgap, and improved charge separation efficiency. Characterization results confirmed successful Ag incorporation, which promoted effective reactive oxygen species generation. In this study, a silver-doped LaCoO₃ photocatalyst was synthesized via a co-precipitation method and evaluated for the visible-light-driven degradation of amikacin. Results demonstrate that Ag doped LaCoO₃ exhibits 94% degradation towards Amikacin.

Keywords: Rare earth element, Silver, Photocatalyst, Co-precipitation, Degradation, Visible light.

| PP-91 |

Degradation of Antibiotic using Cu-Al Co-doped MnO₂ Nanocomposite

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Abstract

Antibiotics are widely used pharmaceutical compounds for the treatment of bacterial infections in humans and animals. However, excessive and improper use has led to their continuous release into water bodies through hospital, domestic, and industrial waste water. Cu-Al co-doped MnO₂ nanoparticles were successfully synthesized by a Co-precipitation method and characterized using FT-IR, UV-DRS, XRD, XPS and FESEM techniques. The XRD pattern confirmed the tetragonal phase of MnO₂. FT-IR analysis showed the characteristic Mn–O vibrations at 600 cm⁻¹. UV–DRS studies were revealed the enhanced visible-light absorption with a reduced band gap of approximately 2.2 eV due to co-doping. The photocatalytic activity was evaluated for ciprofloxacin (30mg/L) degradation under sunlight irradiation, achieving about 94% degradation within 60 minutes. The results demonstrate that Cu–Al co-doped MnO₂ is a promising and efficient photocatalyst for the removal of antibiotic contaminants from wastewater under sunlight irradiation.

Keywords: Wastewater treatment, Ciprofloxacin degradation, Cu–Al co-doping, MnO₂ and precipitation.

| PP-92 |

Sulfur–Phosphorus Co-Doped Carbon Dots for Turn-Off Fluorescence Detection of Chloramphenicol

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Abstract

Sulfur–phosphorus co-doped carbon dots (S,P-CDs) were synthesized via a green one-step hydrothermal method using beetroot extract as a renewable carbon source, with urea, thiourea, and phosphoric acid as heteroatom precursors. Hydrothermal treatment at 180 °C for 6 h produced highly water-dispersible S,P-CDs with strong blue fluorescence (emission 440 nm at 360 nm excitation) and a quantum yield of 29.8%. Transmission electron microscopy showed uniformly distributed nanoparticles (~3.6 nm), while FTIR and XPS confirmed successful S and P doping and abundant surface functional groups. The S,P-CDs exhibited excellent photostability, salt tolerance, and pH stability. Notably, fluorescence was selectively enhanced in the presence of chloramphenicol (CAP) due to suppression of non-radiative recombination via specific CD–CAP interactions. A linear relationship between fluorescence enhancement (F/F_0) and CAP concentration was obtained from 0.08–20.0 μM , with a detection limit of 22 nM ($S/N = 3$). The probe showed high selectivity over common metal ions, amino acids, and other antibiotics, and was successfully applied to spiked real samples with recoveries of 95.8–103.6% and RSDs below 4.3%. These results demonstrate a simple, sensitive, and eco-friendly method for rapid CAP monitoring.

Keywords: Sulfur–phosphorus co-doped carbon dots, Chloramphenicol detection, Turn-off fluorescence sensor, Green synthesis, Real sample analysis

| PP-93 |

Synthesis and Characterizations of V₂O₅/FeOOH Composite Photocatalyst

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Abstract

Vanadium pentoxide (V₂O₅)-based composites have considerable interest in applications such as catalysts and electrode materials. In this paper, V₂O₅/iron oxyhydroxide (FeOOH) composite was prepared to explore its photocatalytic application in wastewater treatment. First, V₂O₅ was prepared by using thermal decomposition method. Hydrolysis method was used to prepare FeOOH in presence of V₂O₅. The resultant V₂O₅/FeOOH was characterized by different analytical techniques. The formation of V₂O₅ crystals and FeOOH were confirmed by powder X-ray diffraction analysis. The occurrence of V-O, and Fe-O (metal - oxygen) in V₂O₅/FeOOH composite was determined by Fourier transform (FTIR) infrared spectroscopy. V₂O₅/FeOOH composite shows absorption from UV to visible light region. The band gap of V₂O₅/FeOOH composite was calculated by using Tauc plot method. The catalytic properties of V₂O₅/FeOOH composite were examined by using hydrogen peroxide (H₂O₂)-mediated photodegradation of Congo red (anionic) and methylene blue (cationic) and in water medium under visible light irradiation. The as-prepared V₂O₅/FeOOH composite showed photocatalytic activity under the optimized experimental condition and it is expected to become a great catalyst in the H₂O₂-assisted photocatalytic treatment of dye contaminated water.

Keywords: V₂O₅/FeOOH, Composite, Photocatalysis, H₂O₂, Congo red, Methylene blue.

| PP-94 |

Metal-Free Fluorescent Recognition of Glyphosate Using Biomass-Derived Nitrogen-Doped Carbon Dots

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Abstract

Carboxyl-rich nitrogen-doped carbon dots (N-CDs) were synthesized via a green one-step hydrothermal method using lemon juice and urea as sustainable carbon and nitrogen precursors. The hydrothermal treatment at 180 °C for 6 h produced highly water-dispersible N-CDs exhibiting strong blue fluorescence with an emission maximum at 445 nm under 360 nm excitation and a quantum yield of 31.2%. Transmission electron microscopy revealed uniformly distributed nanoparticles with an average size of ~3.4 nm, while FTIR and XPS analyses confirmed abundant surface carboxyl groups and successful nitrogen doping. The as-prepared N-CDs showed excellent photostability, salt tolerance, and pH stability. Owing to the strong hydrogen bonding and electrostatic interactions between glyphosate molecules and the carboxyl-rich surface of N-CDs, the fluorescence intensity was efficiently quenched through an aggregation-induced quenching mechanism. Under optimized conditions, a good linear relationship was obtained between the fluorescence quenching ratio (F_0/F) and glyphosate concentration in the range of 0.02–15.0 μM , with a low limit of detection of 9.5 nM ($S/N = 3$). The proposed metal-free sensing platform exhibited high selectivity toward glyphosate over common metal ions, anions, amino acids, and other coexisting pesticides. The method was successfully applied to the determination of glyphosate in spiked river and tap water samples, achieving satisfactory recoveries of 96.4–103.1% with relative standard deviations below 4.0%. These results demonstrate that the lemon-juice-derived N-CDs provide a simple, low-cost, and environmentally friendly strategy for ultrasensitive and metal-free fluorescence monitoring of glyphosate in environmental samples.

Keywords: Nitrogen-doped carbon dots, Glyphosate sensing, Aggregation-induced quenching, Green synthesis, Metal-free fluorescence sensor.

| PP-95 |

Synthesis and Characterization of Ni₃V₂O₈/Co-Cu LDH Nanocomposite for Supercapacitor Applications

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Abstract

Supercapacitors have attracted significant attention as efficient energy storage devices, due to their high-power density and long cycle life. In this work, a binder-free Ni₃V₂O₈/Co-Cu layered double hydroxide (LDH) composite electrode was successfully synthesized directly on nickel foam via a two-step hydrothermal process. X-ray diffraction (XRD) analysis confirmed the formation of crystalline Ni₃V₂O₈ and Co-Cu LDH phases, indicating successful composite formation. X-ray photoelectron spectroscopy (XPS) revealed the presence of Ni, Co, Cu, V, and O with multiple oxidation states, confirming the redox-active nature of the electrode. Scanning electron microscopy (SEM) showed a porous, interconnected 3D-flower structure morphology that provides high surface area and facilitates rapid ion transport. Electrochemical studies demonstrated good redox behaviour, and the electrode delivered a specific capacitance of 1141 F g⁻¹ at 1 A g⁻¹ with stable performance. These results highlight the potential of the Ni₃V₂O₈/Co-Cu LDH composite as a promising electrode material for supercapacitor applications.

Keywords: Ni₃V₂O₈; Co-Cu LDH; Hydrothermal, Supercapacitor, Energy storage

| PP-96 |

Green-Synthesized Oxygen-Rich Carbon Dots for Enzyme-Free Fluorescence Detection of Organophosphate Pesticides through Hydrolysis-Induced Response

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Abstract

Oxygen-rich carbon dots (O-CDs) were prepared via a green hydrothermal carbonization route using pesticide-free cauliflower juice as a renewable carbon precursor. The hydrothermal treatment at 180 °C for 6 h produced highly water-dispersible O-CDs exhibiting strong blue fluorescence with an emission maximum at 440 nm under 360 nm excitation and a quantum yield of 27.6%. Transmission electron microscopy showed uniformly distributed nanoparticles with an average diameter of ~3.9 nm, while FTIR and XPS analyses confirmed the presence of abundant oxygen-containing functional groups (–OH, –COOH, and C=O) on the surface. The O-CDs displayed excellent photostability, good salt tolerance, and stable fluorescence over a wide pH range. Based on the hydrolysis of organophosphate pesticides and the subsequent interaction of hydrolysis products with the oxygen-rich surface of the O-CDs, a distinct and concentration-dependent fluorescence response was observed, enabling enzyme-free detection. Under optimized conditions, the fluorescence response exhibited good linearity toward organophosphate pesticides in the range of 0.05–20.0 μM, with a low limit of detection of 21 nM (S/N = 3). The sensing system showed high selectivity against common ions and potential interfering substances. The practical applicability of the method was demonstrated by the determination of organophosphate residues in spiked tap water and vegetable samples, affording recoveries of 96.3–103.8% with relative standard deviations below 4.6%. The proposed biomass-derived O-CD-based platform provides a simple, low-cost, and environmentally friendly strategy for enzyme-free fluorescence monitoring of organophosphate pesticides

Keywords: Carbon dots, Organophosphate pesticides, Enzyme-free fluorescence sensing, Greensynthesis, Biomass-derived nanomaterials

| PP-97 |

Development of Biodegradable Film for Advanced Wound Dressing and Wound Healing Applications

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Abstract

The growing demand for sustainable and biologically active wound care materials has driven the development of biodegradable polymeric nanocomposites as alternatives to conventional synthetic wound dressings. In this study, a novel biodegradable nanoparticle-reinforced wound dressing film was fabricated using egg white protein and aloe vera gel as natural biopolymers for film-forming ability and structural stability. Silica (SiO₂) nanoparticles were introduced as inorganic nano-reinforcement to enhance mechanical strength and functional performance. The nanocomposite films were prepared through solution casting technique under acidic conditions to promote protein denaturation and intermolecular cross-linking within the polymeric matrix. Fourier Transform Infrared Spectroscopy (FTIR) analysis confirmed strong intermolecular hydrogen bonding interactions among hydroxyl (–OH), amide (–CONH–), and silanol (Si–OH) functional groups, indicating effective integration of SiO₂ nanoparticles into the biopolymer network. X-ray Diffraction (XRD) analysis revealed a semi-crystalline structure with characteristic diffraction peaks corresponding to amorphous silica nanoparticles, demonstrating improved structural organization and nanoparticle dispersion within the matrix. Field Emission Scanning Electron Microscopy (FESEM) images showed uniform surface morphology with well-dispersed SiO₂ nanoparticles and reduced agglomeration, contributing to enhanced surface smoothness and minimized crack formation. The incorporation of nanoparticles improved film integrity, transparency, and mechanical robustness compared to the non-reinforced film. We are anticipating that the synergistic interaction between natural biopolymers and inorganic nanofillers results a biodegradable, flexible, and structurally stable composite with potential antimicrobial activity, moisture retention capability, and enhanced wound dressings and wound healing performance. This study presents a cost-effective, eco-friendly, and scalable strategy for developing multifunctional protein-based nanocomposites suitable for advanced biomedical wound dressing and wound healing applications.

Keywords: Flim, Wound dressings, Wound healing, Egg white, Aloe Vera, Silica.

| PP-98 |

Crystallographic Studies of Metal Complex using Heterocyclic and Organic Acids

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Abstract

This presentation delves into the crystallographic study of novel metal complexes created by combining heterocyclic compounds and organic acids. Metal complexes derived from these ligands are well known for their versatile and useful properties in a variety of fields, including medicine and catalysis. Our findings describe a systematic approach to synthesizing these complexes via slow evaporation. Following synthesis, the complexes are thoroughly characterized using advanced spectroscopic techniques such as infrared (IR), ultraviolet-visible (UV-Vis), nuclear magnetic resonance (NMR), and X-ray diffraction (XRD) to determine their structural properties. Despite the well-known utility of such complexes, more research is needed to clearly link their intricate structures to their observed activities. By creating, synthesizing, and spectroscopically analyzing metal complexes involving heterocyclic ligands and organic acids like salicylic acid, this work seeks to close this gap. It is believed that the produced metal complexes have a great deal of potential for use in medicinal chemistry. Furthermore, the study investigates their broader utility in fields such as catalysis and material science, emphasizing the versatility and significance of these novel compounds. This presentation provides a comprehensive overview of our findings, focusing on the structural elucidation and potential applications of these fascinating metal complexes, paving the way for future advances in a variety of scientific disciplines.

| PP-99 |

Structural and Electrochemical Insights into $\text{Ce}_2(\text{WO}_4)_3/\text{g-C}_3\text{N}_4$ Nanocomposites for Enhanced Supercapacitor Performance

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Abstract

Cerium tungstate ($\text{Ce}_2(\text{WO}_4)_3$) is a rare-earth metal tungstate known for its excellent structural stability, wide band gap, and attractive physicochemical properties. Its unique crystal framework and high thermal stability make it a promising candidate for advanced energy-storage applications. In this work, $\text{Ce}_2(\text{WO}_4)_3/\text{g-C}_3\text{N}_4$ nanocomposites were successfully synthesized using a simple hydrothermal method to investigate their potential for high-performance supercapacitor applications. X-ray diffraction (XRD) analysis confirmed the formation of crystalline $\text{Ce}_2(\text{WO}_4)_3$ and its effective integration with $\text{g-C}_3\text{N}_4$. FTIR spectra validated the characteristic bonding features of both components, indicating successful composite formation. FE-SEM analysis revealed a uniformly distributed nanostructure with enhanced surface morphology, facilitating efficient electrolyte ion diffusion and rapid charge transfer. Electrochemical studies demonstrated improved specific capacitance, excellent rate capability, and superior cycling stability compared to the individual constituents. The synergistic interaction between $\text{Ce}_2(\text{WO}_4)_3$ and $\text{g-C}_3\text{N}_4$ significantly enhances the overall electrochemical performance, making the nanocomposite a promising electrode material for next-generation supercapacitor devices.

Keywords: Cerium tungstate ($\text{Ce}_2(\text{WO}_4)_3$)/ $\text{g-C}_3\text{N}_4$, Nanocomposite, Hydrothermal synthesis, Supercapacitor, Energy storage application.

| PP-100 |

Synthesis of Electrical and Morphological Analysis of Poly (*m*-Phenylenediamine)/CuMnFe₂O₄

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Abstract

In this study, poly(*m*-phenylenediamine) (PmPD)/CuMnFe₂O₄ nanocomposites were successfully prepared using an in-situ chemical oxidative polymerisation method. The CuMnFe₂O₄ nanoparticles were first synthesised through a sol-gel auto-combustion process and then incorporated into the polymer matrix to enhance its overall properties. The main goal of this work was to improve the structural, magnetic, thermal, and dielectric characteristics of the polymer by introducing ferrite nanoparticles. Powder X-ray diffraction analysis confirmed the formation of the crystalline spinel structure of CuMnFe₂O₄ (NPs) and showed that the nanoparticles were successfully embedded within the PmPD matrix without altering their phase. The crystallite size was estimated using the Debye–Scherrer equation. Fourier Transform Infrared spectroscopy further verified the formation of the nanocomposites by identifying both the characteristic metal–oxygen vibrations of ferrite and the functional groups of the polymer. Field Emission Scanning Electron Microscopy images revealed a mainly spherical morphology with good dispersion of nanoparticles in the polymer matrix. Magnetic studies demonstrated ferromagnetic behaviour, while thermogravimetric analysis showed improved thermal stability with higher ferrite content. Dielectric measurements indicated frequency-dependent behaviour, highlighting the potential of these nanocomposites for electronic and energy storage applications.

Keywords: CuMnFe₂O₄, PmPD, Spinel ferrite, Sol–gel auto-combustion, Dielectric properties.

| PP-101 |

Synergistic Effect of Co_3O_4 Loaded $\text{g-C}_3\text{N}_4/\text{Bi}_2\text{MoO}_6$ Ternary Heterojunction S-Scheme Photocatalytic degradation of Malachite Green

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Abstract

Co_3O_4 loaded $\text{g-C}_3\text{N}_4/\text{Bi}_2\text{MoO}_6$ ternary nanocomposite was successfully synthesized via a hydrothermal method followed by calcination for visible-light photocatalytic applications. Powder X-ray diffraction (XRD) analysis confirmed the crystalline Bi_2MoO_6 and $\text{g-C}_3\text{N}_4$ phases along with well-dispersed Co_3O_4 , indicating the successful formation of a ternary nanocomposite with strong interfacial interaction and no impurity phases. Scanning electron microscopy (SEM) revealed improved surface morphology and intimate contact among the components, while energy-dispersive X-ray spectroscopy (EDX) verified the presence of Bi, Mo, O, C, N, and Co elements. X-ray photoelectron spectroscopy (XPS) further confirmed the chemical states of Bi^{3+} , Mo^{6+} , and $\text{Co}^{2+}/\text{Co}^{3+}$, demonstrating effective electronic interaction within the composite. The incorporation of Co_3O_4 facilitates the formation of an internal electric field between $\text{g-C}_3\text{N}_4$ and Bi_2MoO_6 , promoting efficient charge separation and suppressing electron-hole recombination. Consequently, the ternary nanocomposite exhibited significantly enhanced visible-light-driven photocatalytic degradation of malachite green, making it a promising candidate for wastewater treatment applications.

Keywords: Co_3O_4 -Loaded $\text{g-C}_3\text{N}_4/\text{Bi}_2\text{MoO}_6$, Ternary composite, Visible-light photocatalysis, Malachite green, S-Scheme mechanism.

| PP-102 |

Synthesis of Ivacaftor and Its Key Starting Material Using a Flow Process

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Abstract

Cystic Fibrosis (CF) is a chronic, life-threatening genetic disorder caused by mutations in the Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) gene, affecting an estimated 100,000 to 200,000 individuals across 94 countries. While Ivacaftor remains a primary therapeutic intervention, its high cost often limits patient access, particularly in low- and middle-income countries. In this study, we report the streamlined synthesis of the Ivacaftor Active Pharmaceutical Ingredient (API) and its Key Starting Materials (KSMs) using an advanced micro-flow reactor system. By transitioning to a continuous flow process, we demonstrate significant improvements in synthesis time, product yield, and chemical purity. This approach provides a scalable and cost-effective manufacturing alternative to traditional batch synthesis, ultimately aiming to reduce the economic burden of CF treatment globally.

Keywords: Cystic fibrosis, API, KSMs

| PP-103 |

Hierarchical Heterostructure of NiMoO₄ as an Efficient Electrocatalyst for Water Splitting

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Abstract

Efficient and cost-effective electrocatalysts are essential for sustainable hydrogen production through water splitting. In this work, a hierarchical NiMoO₄/Co-Cu layered double hydroxide (LDH)/MXene ternary composite was rationally designed and synthesized as a bifunctional electrocatalyst. NiMoO₄ nanostructures were first grown via a hydrothermal route followed by annealing to improve crystallinity and electrical conductivity. Subsequently, Co-Cu LDH nanosheets were uniformly deposited onto the NiMoO₄ surface to provide abundant redox-active sites and a layered morphology. Finally, conductive MXene sheets were integrated to construct a three-dimensional (3D) interconnected framework, enhancing charge transport, interfacial contact, and structural stability. The synergistic combination of transition metal oxide, LDH, and MXene promotes rapid electron transfer, increased active surface area, and efficient ion diffusion. This rationally engineered architecture offers a promising strategy for developing high-performance, durable electrocatalysts for overall water splitting applications.

Keywords: NiMoO₄/Co-Cu LDH/MXene, Hydrothermal synthesis, Spinel nanostructures, Water splitting applications.

| PP-104 |

Core-shell Structured Tungsten Disulfide/Zeolitic Imidazolate Framework-67 Nanocomposites as Cathode Material for Supercapacitor Application

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Abstract

Metal-organic frameworks and their composites are widely used in the energy and environmental sectors because of their larger surface areas, porous nature and electroactive organic counterparts. A simple *in-situ* growth is employed for designing a heterostructure composite using zeolitic imidazolate framework-67 with tungsten disulphide (WS₂). The prepared WS₂@ZIF-67 composites have been evaluated using HR-TEM, XPS, and BET studies to evaluate their structural, morphological, chemical compositions and porous nature. The electrochemical performance was investigated with KOH and redox additive electrolyte (RAE) in a three-electrode configuration. The specific capacitances were found to be 625.32 and 1256.89 F g⁻¹ for KOH and RAE. The nanocomposite electrode has excellent cyclic stability, with 81.95% capacity retention after 6000 cycles. The constructed asymmetric device (WS₂@ZIF-67)//AC demonstrated good capacitive performance over a broad potential window of 0 to 1.7 V, achieving a specific capacitance of 66.58 F g⁻¹ and capacitance retention of 89.72%. The designed ASC device has series resistance values of 0.452 Ω and 0.653 Ω before and after 10,000 GCD cycles.

Keywords: Zeolitic imidazolate framework-67; Core-shell; Energy storage; Charge-discharge; Capacity retention

| PP-105 |

Fast Modification of Porous Nickel Foam Substrate as Anode Material for Anion Exchange Membrane Water Electrolysis

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Abstract

The urgent need for sustainable energy solutions has driven research into efficient hydrogen production technologies. Anion exchange membrane water electrolysis (AEMWE) offers a promising pathway, but its efficiency is limited by the sluggish kinetics of the oxygen evolution reaction (OER). In this work, a simple and rapid FeCl₃ etching strategy was employed to modify porous nickel foam substrates, enabling the incorporation of Fe species and subsequent formation of NiFe hydroxides under alkaline conditions. Systematic variation of FeCl₃ concentration and etching duration revealed that the optimized Ni-FeCl₃ (0.1 M, 3 h) electrode exhibited superior OER activity, delivering a low overpotential of 263 mV at 10 mA cm⁻² and a reduced Tafel slope of 100 mV dec⁻¹. Electrochemical surface area analysis confirmed enhanced active site exposure, while chronopotentiometry demonstrated excellent stability with minimal voltage decay over extended operation. When integrated into an AEMWE, the Ni-FeCl₃ (0.1 M, 3 h) anode paired with bare Ni foam cathode achieved a current density of 0.5 A cm⁻² at a cell voltage of 1.85 V, outperforming the unmodified Ni foam configuration by 430 mV. Long-term testing over 50 hours validated the durability of the etched substrate, with only 5.58% performance decay. These findings highlight FeCl₃ etching as a cost-effective and scalable strategy for fabricating high-performance anodes, offering significant potential for practical hydrogen generation in sustainable energy systems.

Keywords: FeCl₃-etched Ni foam anodes, Oxygen evolution reaction (OER) enhancement, Anion exchange membrane water electrolysis (AEMWE)

| PP-106 |

Degradation of Antibiotic using Ag-Mn co-doped NiO Nanocomposite

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Abstract

Water pollution is caused by antibiotics has resulted in a threat to living organisms, animals and humans, hence there is a need to synthesize multifunctional materials that can be used for the degradation of various pollutants. In this study was to Ag Mn co-doped NiO Nano composites and test this material for photocatalytic degradation. The synthesized Nano composites was characterised using UV-DRS, FTIR, XRD, XPS and Fe-SEM. The material was tested for its photocatalytic efficiency against antibiotic Oflaxacin. XRD confirmed the formation of Ag Mn co-doped NiO. UV-DRS analysis showed a strong absorption peak at 276 nm, corresponding to an optical band gap energy of approximately 4.49 eV. The Ag Mn co-doped NiO was demonstrated using FTIR. From the surface analysis, the morphology of the synthesized Nano composites was found to be crystalline cubic. Against Oflaxacin, a 80% degradation was observed within 60mins. These results show that at optimum conditions, these materials are able to degrade various pollutants in wastewater.

Keywords: Wastewater treatment, Oflaxacin degradation, Ag&Mn co-doped NiO, Co-precipitation method, Photocatalysis

| PP-107 |

High-Energy Solid-State Synthesis of Sodium Manganese Oxide Nanobelts with Enhanced Electrochemical Performance

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Abstract

With the increasing demand for clean and affordable energy storage, sodium-based supercapacitors have emerged as promising candidates due to their low cost, environmental compatibility, abundance, and long-term stability. In this study, Na_{0.70}MnO_{2.05} nanoparticles were synthesized via a high-energy solid-state ball milling technique, forming a hexagonal crystal structure. FESEM and HRTEM analyses revealed the surface morphology, showing nanobelt structures with polycrystalline characteristics and a uniform elemental distribution of Na, Mn, and O. XPS analysis confirmed the presence of Mn³⁺/Mn⁴⁺ oxidation states, providing multiple active sites. Thermogravimetric analysis demonstrated that the material maintained high thermal stability up to 1000 °C, with negligible mass loss beyond 700 °C. Electrochemical performance of the prepared Na_{0.70}MnO_{2.05} as a working electrode has been compared in 1 M pure NaOH electrolyte and redox-modified electrolytes (NaOH + 0.1 M KI, and NaOH + 0.1 M K₃[Fe(CN)₆]) in three-electrode configurations. The Na_{0.70}MnO_{2.05} electrode delivered a maximum specific capacitance of 2682.5 F g⁻¹ at 4 A g⁻¹ in the redox additive electrolyte made of 1 M NaOH and 0.1 M K₃[Fe(CN)₆] electrolyte. In comparison, the Na_{0.70}MnO_{2.05} electrode achieved 932.4 F g⁻¹ at 2 A g⁻¹ in 1 M NaOH + 0.1 M KI, and 122.16 F g⁻¹ at 0.5 A g⁻¹ in 1 M NaOH electrolytes. The remarkable capacitance enhancement in the presence of redox additives may be due to the supplementary faradaic-active species and the increased ionic transport by additional redox species, synergistically facilitating rapid ion exchange at the electrode–electrolyte interface. Owing to their scalable synthesis, material abundance, and good electrochemical characteristics, these materials are suitable for further development in sustainable energy storage.

Keywords: Sodium Manganese Oxide, Na ion supercapacitor, Redox additive electrolytes.

| PP-108 |

Ultrasonic waves triggered CeO₂-hBN-g-C₃N₄ heterojunction nanocomposites as a multifunctional electrode material for asymmetric supercapacitor and photocatalytic applications

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Abstract

Addressing the dual challenges of energy scarcity and water contamination requires the development of high-performance multifunctional nanomaterials. In this work, a CeO₂-h-BN-g-C₃N₄ ternary nanocomposite was fabricated through a hydrothermal process followed by ultrasonic treatment. Phase formation and vibrational features were confirmed using XRD and FTIR analyses, while optical properties were evaluated by UV-Vis absorption and fluorescence spectroscopy. Surface morphology and elemental composition were examined by SEM-EDAX and HRTEM, with XPS and BET providing insights into surface states and textural characteristics. Electrochemical studies (CV, GCD, and EIS) revealed remarkable charge-storage behaviour, confirming its suitability as a stable supercapacitor electrode material. The asymmetric device assembled with CeO₂-h-BN-g-C₃N₄ //activated carbon electrodes demonstrated an energy density of 36.67 Wh kg⁻¹ and a power density of 825 W kg⁻¹. Notably, the device retained 84.2 % of its efficiency after 5000 cycles. Furthermore, when employed as a photocatalyst for the degradation of methylene blue dye under visible light irradiation, the CeO₂-h-BN-g-C₃N₄ composite achieved a degradation efficiency of 99.6 %, outperforming all other synthesized samples. These results highlight CeO₂-h-BN-g-C₃N₄ as a versatile material with significant potential for both energy storage and environmental purification.

Keywords: Smart nanomaterial, Electrode, Advanced oxidation process, Synergistic effect

| PP-109 |

Green Synthesis of NiO and CuO Nanoparticles Using *Vitis vinifera* Extract for Photocatalytic Activity

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Abstract

Green synthesis of nickel oxide (NiO) and copper oxide (CuO) nanoparticles was carried out using *Vitis Vinifera* peel extract as a natural reducing and stabilizing agent. The phytochemicals present in the grape peel facilitate an eco-friendly, cost-effective synthesis without the use of toxic chemicals. The synthesized nanoparticles were characterized using various analytical techniques to confirm their structural and optical properties. The photocatalytic activity of NiO and CuO nanoparticles was evaluated through the degradation of organic dye under light irradiation. Among these, CuO nanoparticles exhibited higher photocatalytic efficiency due to improved charge separation and surface activity, indicating their potential application in wastewater treatment.

Keywords: Green synthesis, *Vitis Vinifera* peel extract, Nickel Nitrate, Copper Nitrate, NiO nanoparticles, CuO nanoparticles, Photocatalytic degradation, Organic dye removal.

| PP-110 |

Plant-Mediated Synthesis of ZnO, CuO and NiO Nanoparticles Using Cinnamon Extract and Investigation of Their Photocatalytic Efficiency

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Abstract

In this study, a facile, sustainable and eco-friendly green synthesis route was employed for the preparation of ZnO, CuO and NiO nanoparticles using cinnamon extract as a natural reducing and stabilizing agent. Metal nitrates, namely zinc nitrate ($\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$), copper nitrate ($\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$) and nickel nitrate ($\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$), were used as precursor salts, while water served as the solvent. The synthesis was carried out under controlled conditions to promote efficient nanoparticle formation. The phytochemicals present in cinnamon extract played a crucial role in reducing metal ions and stabilizing the formed nanoparticles. The prepared nanoparticles were systematically characterized to evaluate their structural, morphological, thermal, chemical and optical properties using X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), high-resolution transmission electron microscopy (HR-TEM), energy-dispersive X-ray spectroscopy (EDX), Fourier transform infrared spectroscopy (FT-IR) and UV-Visible spectroscopy. The results confirmed the successful formation of crystalline metal oxide nanoparticles with distinct surface morphologies and optical band gap energies. The photocatalytic performance of ZnO, CuO and NiO nanoparticles was comparatively investigated under light irradiation. Variations in photocatalytic efficiency were observed, which can be attributed to differences in band gap energy, surface area and charge carrier recombination rates. The findings reveal that cinnamon-mediated metal oxide nanoparticles exhibit promising photocatalytic activity, highlighting their potential application in environmental remediation and wastewater treatment.

Keywords: Green synthesis, Cinnamon extract, Metal oxides, Photocatalysis, Environmental remediation.

| PP-111 |

Green Synthesis of N/B Co-Doped Carbon Dots as π - π Stacking-Responsive Fluorescent Probes for Sensitive Detection of Carbendazim

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Abstract

Boron self-doped carbon dots (B-CDs) were synthesized via a simple and green hydrothermal route using a biomass-derived precursor, yielding highly water-dispersible nanodots with strong blue fluorescence. The as-prepared B-CDs exhibit an emission maximum at 440 nm under 360 nm excitation and a quantum yield of 27.3%. Transmission electron microscopy revealed uniformly distributed nanoparticles with an average size of ~ 3.6 nm, while FTIR and XPS analyses confirmed successful boron self-doping and the presence of abundant surface functional groups. The B-CDs show excellent photostability, salt tolerance, and pH stability. Owing to strong π - π stacking interactions between carbendazim (CBZ) and the aromatic domains of the B-CDs, the fluorescence intensity is efficiently quenched in a concentration-dependent manner, enabling sensitive detection. Under optimized conditions, a good linear relationship was obtained between the fluorescence quenching ratio (F_0/F) and CBZ concentration in the range of 0.02–20.0 μM , with a low limit of detection of 11 nM ($S/N = 3$). The sensing system exhibited high selectivity toward CBZ over common metal ions, anions, and other pesticides. The method was successfully applied to the determination of CBZ in spiked water and agricultural samples, achieving satisfactory recoveries of 95.8–103.2% with relative standard deviations below 4.0%. These results demonstrate that the B-CD-based fluorescent probe provides a simple, sensitive, and environmentally friendly platform for monitoring carbendazim residues in real samples.

Keywords: Boron-doped carbon dots, Carbendazim detection, Fluorescence sensing, π - π stacking interaction, Real sample analysis

| PP-112 |

Bismuth Oxyhalides as Active Photocatalyst for Degradation of Methylene Blue under UV Light Irradiations

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Abstract

Bismuth oxybromide (BiOBr), a layered semiconductor with a unique internal electric field, has attracted significant attention as an efficient photocatalyst for environmental remediation. In this study, BiOBr-based photocatalysts were synthesized via Hydrothermal method and evaluated for the degradation of methylene blue (MB) dye under ultraviolet UV light irradiation. The prepared photocatalyst was characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and UV–Vis diffuse reflectance spectroscopy (DRS) to investigate its crystalline structure, morphology, and optical properties. The results confirmed the formation of well-crystallized BiOBr with a suitable band gap for photocatalytic applications. Photocatalytic experiments demonstrated that the prepared BiOBr photocatalyst exhibits 97% degradation efficiency towards methylene blue under UV light irradiation. The photocatalyst also showed good stability and reusability over multiple cycles without significant loss in activity.

Keywords: Bismuthoxybromide, Photocatalyst, Methylene blue degradation.

| PP-113 |

Non-stabilized Azomethine Ylides in the Claisen Condensation: Synthesis of 5-Isatinylidenerhodanine Derivatives

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Abstract

Active methylene compounds react with *in situ* generated nonstabilized azomethine ylides (generated from substituted isatins and sarcosine) via the domino Claisen condensation to form 5-isatinylidenerhodanine derivatives. When the starting material possesses a single activated hydrogen, the reaction terminates at the Claisen condensation stage. The developed methodology was applied to a short and efficient synthesis of 5-isatinylidenerhodanine derivatives. The regiochemistry and structures of the 5-isatinylidenerhodanine derivatives were determined with FT-IR, ¹H NMR, ¹³C NMR and 2D NMR spectroscopic data and mass spectral analysis.

Keywords: 5-Isatinylidenerhodanine, Claisen condensation, NMR, Mass spectral analysis.

| PP-114 |

Advanced Cathode Materials for Aluminum-Air Batteries: Metal Oxide/Activated Carbon Composites – A Comprehensive Review

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Abstract

Aluminum-air (Al-air) batteries represent a promising next-generation energy storage platform, owing to their superior theoretical energy density, the abundance and low cost of aluminum, and inherent safety features. Nevertheless, commercialization remains hindered by challenges, particularly the sluggish oxygen reduction reaction (ORR) kinetics at the air cathode. Although platinum-based catalysts demonstrate exceptional activity, their scarcity and expense underscore the need for cost-effective alternatives. This review evaluates advancements in metal oxide (MO_x)/activated carbon (AC) composites as efficient ORR electrocatalysts for Al-air battery cathodes. Activated carbon serves as a porous, conductive, and economical substrate, whereas metal oxides—such as MnO₂, Co₃O₄, Fe₂O₃, and mixed-metal variants—furnish active catalytic sites for oxygen reduction. The synergistic interplay between these constituents is scrutinized: the AC framework promotes uniform dispersion and accessibility of MO_x nanoparticles, enhances mass transport, and bolsters electrical conductivity, with MO_x providing the principal catalytic activity. Synthesis approaches, including impregnation, hydrothermal processes, and pyrolysis of precursors, are delineated, accompanied by essential characterization methods. Performance enhancements in Al-air batteries—manifested in elevated discharge voltage, specific capacity, and power density—are systematically analyzed. Persistent challenges, such as catalyst durability and conductivity, are highlighted, alongside prospective research avenues encompassing refined synthesis techniques, defect engineering, and holistic system integration to expedite viable Al-air battery deployment.

Keywords: Aluminum-air battery, oxygen reduction reaction, metal oxides.

| PP-115 |

Preparation and Characterization of a Composite made up of ZnO and Carbon obtained from Banana Peel as an Electrocatalyst for Aluminum-Air Battery

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Abstract

This investigation presents the eco-conscious synthesis of a zinc oxide–carbon (ZnO–C) composite wherein the carbon was derived from banana peel biomass via KOH chemical activation at 600 °C. Comprehensive characterization using X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), and Energy-Dispersive X-Ray Spectroscopy (EDX) confirms the successful incorporation of crystalline ZnO nanoparticles within an amorphous carbon matrix. Fourier-transform infrared (FTIR) spectroscopy reveals the decomposition of organic volatiles originating from the biomass and substantiates the in-situ formation of ZnO embedded in the carbon framework. Electrochemical evaluation highlights the composite's excellent capacitive behavior, demonstrating a maximum specific capacitance of 1212 F g⁻¹ at a scan rate of 10 mV s⁻¹, which decreases to 380 F g⁻¹ at 100 mV s⁻¹ attributable to restricted ion diffusion at elevated scan rates. Galvanostatic charge–discharge (GCD) measurements exhibit pronounced asymmetry and an extended discharge plateau centered around 1.75 V, indicative of the redox activity of ZnO and the contribution of oxygen-containing functional groups in the carbon matrix. Electrochemical impedance spectroscopy (EIS) Nyquist analysis reveals a moderate charge transfer resistance of approximately 68.2 Ω, along with characteristic Warburg diffusion behavior, signifying efficient ion transport promoted by the composite's hierarchical porous architecture. Collectively, these results underscore the potential of banana peel-derived ZnO–carbon composites as sustainable and high-performance electrocatalyst materials for aluminum–air batteries.

Keywords: Biomass-derived activated carbon; Banana peel; KOH activation; ZnO–carbon composite; Oxygen reduction reaction (ORR); Aluminum–air battery; Sustainable energy storage.

| PP-116 |

Synthesis, Structural Elucidation, Intermolecular and Non-Covalent Interaction Analysis, and Molecular Docking Studies of 3-Chloro-3-methyl-2,6-bis(4-methoxyphenyl)piperidin-4-one Picrate (CMMyPP)

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Abstract

In this article, we discuss the synthesis, electronic structure, and theoretical calculations of 3-chloro-3-methyl-2,6-bis(4-methoxyphenyl)piperidin-4-one picrate (CMMyPP). We synthesized the compound and characterized its structure using FT-IR, ¹H NMR, and ¹³C NMR spectroscopy. We used density functional theory (DFT) at the B3LYP/6-311++G(d,p) level to optimize its geometry and assess electronic properties like frontier molecular orbitals (FMOs). We also estimated the natural bond orbital (NBO), molecular electrostatic potential (MEP), and quantum theory of atoms in molecules (QTAIM). Molecular docking studies were conducted on selected bacterial protein targets linked to necrotizing fasciitis-causing pathogens: *Streptococcus pyogenes* and *Staphylococcus aureus*, using the crystal structures 2PE4 and 4URM, respectively. The docking results show that CMMyPP and its molecular fragments have strong binding affinities to key proteins related to virulence and survival. These binding affinities have docking scores that are comparable to those of standard antibacterial agents.

Keywords: Piperidin-4-one picrate; DFT; NBO; MEP; AIM; Necrotizing Fasciitis

| PP-117 |

Transition Metal–Tuned MoS₂ Nanostructures: Tailoring Structural Integrity and Emerging Optical Prospects

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Abstract

In this study, bare MoS₂, Co-doped MoS₂, and Mn-doped MoS₂ nanostructures were successfully synthesized via a hydrothermal method to investigate the influence of transition metal doping on structural and morphological properties. The crystalline nature and phase purity of the prepared samples were examined using X-ray diffraction (XRD). The diffraction patterns confirmed the formation of hexagonal Molybdenum disulfide without the presence of secondary impurity phases, indicating successful incorporation of Co and Mn ions into the lattice structure. Surface morphology and microstructural features were analyzed using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The images revealed well-defined layered/flower-like nanostructures with uniform distribution. Doped samples exhibited slight morphological variations compared to bare MoS₂, indicating lattice distortion and structural modification induced by the incorporation of transition metals. The study aims to investigate how the incorporation of Co and Mn influences the electronic structure, defect states, vibrational characteristics, and overall physicochemical properties of Molybdenum disulfide. Transition metal doping is known to modify the band structure, induce lattice distortion, and affect charge carrier recombination behavior. Further optical characterization using UV–Visible spectroscopy, FTIR, and photoluminescence (PL) analysis is currently underway to evaluate the impact of dopant incorporation. The combined structural and forthcoming optical studies are expected to provide deeper insight into the suitability of doped MoS₂ for advanced optoelectronic and energy storage applications.

Keywords: Mn/Co-doped Molybdenum disulfide (MoS₂), Hydrothermal synthesis, Nanoflower morphology, Electronic Structure Modification, Optical Characterization.

| PP-118 |

Engineering NiO incorporated MgMoV₂O₆ Cathode material for Efficient Energy Storage Systems

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Abstract

The advancement of sustainable, safe, high performance and low-cost cathode material is essential for next generation storage system. In the present work, Nickel Oxide (NiO) added MgMoV₂O₆ (MMNV) nanocomposite was efficiently synthesized using Sol-gel method to elevate the electrochemical performance of MgMoV₂O₆ (MMV). X-ray diffraction confirms the structural analysis of MgV₂O₆ and MgMoO₄ and cubic NiO phases with an average crystallite size of 16.45 nm confirming the successful integration of NiO into the host matrix. The validation of metal-oxygen bonds is confirmed using FTIR analysis. Along with this SEM studies displayed the uniform morphology of the nanocomposite. Similarly, EDX studies confirms the homogeneous elemental distribution of the nanocomposite in the synthesized material. UV-Vis spectroscopy reveals the optical properties of the MMV and MMNV cathode material indicating reduction in band gap energy to 2.83 eV for (MMNV) to 3.98 eV of (MMV), demonstrating enhanced electronic conductivity and improved charge carrier excitation. Cyclic Voltammetry (CV) analysis evaluates the electrochemical performance and revealed pseudocapacitive behaviour, further Galvanostatic charged is charge (GCD) verifies the reversibility nature of the cathode material. Electrochemical impedance spectroscopy exhibits the dielectric phenomena with reduced charge-transfer resistance for the MMNV electrode, confirms polarization charge transport properties in the composite. Nyquist report displays smaller semicircle for MMNV sample, validating lower interfacial resistance and enhanced ion diffusion. The CV file with quasi-rectangular profile exhibiting distinct redox peaks and GCD profile with symmetric curves confirms hybrid charge storage mechanism with both faradaic and electric double-layer contributions. Hence the present study reveals that integration of NiO considerably enhances the electrical conductivity, thereby improving the structural stability and electrochemical kinetics of MgMoV₂O₆, suggesting the MMNV nanocomposite a potential cathode material for energy storage systems.

Keywords: MgMoV₂O₆, Cathode, Cyclic voltammetry, Electrochemical impedance spectroscopy, Energy storage systems.

| PP-119 |

Fabrication, Characterization and Electrochemical evaluation of Pt-based Cathode Catalysts for Enhanced ORR in PEM Fuel cells

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Abstract

Fuel cells provide a promising, clean-energy solution for power generation across various sectors, thereby acting as a cornerstone of the hydrogen economy. They work on the principle of electrochemical energy conversion, which converts the chemical energy of the fuel (hydrogen) and the oxidizing agent (oxygen) into electricity with water and heat as byproducts. In recent years, fuel cells have emerged as environmentally friendly local power sources, contributing to a sustainable and ecologically balanced future. As a result of the overall production expenses, researchers worldwide are currently focusing on improving the individual components, particularly the catalyst. This research focuses on the fabrication of a highly active carbon-supported platinum-based cathode catalyst for the Polymer Electrolyte Membrane Fuel Cell (PEMFC) applications. A standard proton exchange membrane, such as Nafion is employed to ensure efficient proton conduction and reliable fuel cell performance. Various characterizations like FE-SEM, XRD, XPS and ICP to understand the physical, chemical and structural properties of the synthesized material. Further CV, EIS, LSV studies are used to study the catalytic activity, stability of the fuel cell and its overall electrochemical performances.

Keywords: Fuel cells, Catalyst, PEMFC, Nafion, Structural properties, Electrochemical performance.

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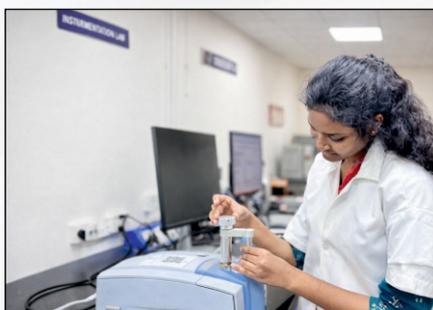
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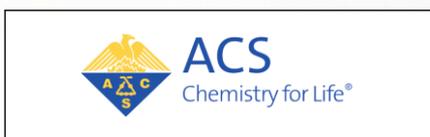


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