



VINAYAKA MISSION'S
KIRUPANANDA VARIYAR
ARTS & SCIENCE COLLEGE



VINAYAKA MISSION'S
RESEARCH FOUNDATION
(Deemed to be University under section 3 of the UGC Act 1956)
(Accredited by NAAC with 'A' Grade & Ranked in NIRF)



iNEEBA 2026

Indo - South Korea - Thailand
6th International e-Conference on
Nanoscience and Nanotechnology for Energy,
Environment and Biomedical Applications
(iNEEBA-2026)

iNEEBA 2026

CONFERENCE PROCEEDINGS

24th & 25th September 2026

Jointly Organized by

VINAYAKA MISSION'S KIRUPANANDA VARIYAR ARTS AND SCIENCE COLLEGE

A Constituent College of Vinayaka Mission's Research Foundation
(Deemed to be University) (Accredited with NAAC 'A' Grade)

In Association with

CORE-FACILITY CENTER FOR
PHOTOCHEMISTRY & NANOMATERIALS,
RESEARCH INSTITUTE OF
ADVANCED CHEMISTRY (RIAC),
GYEONGSANG NATIONAL UNIVERSITY (GNU),
SOUTH KOREA

DEPARTMENT OF
CHEMICAL ENGINEERING,
CHULALONGKORN UNIVERSITY,
THAILAND



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ISBN No :

978-93-344-8849-4



VINAYAKA MISSION'S RESEARCH FOUNDATION

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With the Blessings of

Dr. A. Shanmugasundaram

Founder Chancellor

Vinayaka Mission's Research Foundation, Salem



**VINAYAKA MISSION'S
RESEARCH FOUNDATION**

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With the Benevolence of

Mrs. Annapoorani Shanmugasundaram

**Trustee, Vinayaka Mission's Research Foundation,
Salem**



VINAYAKA MISSION'S RESEARCH FOUNDATION

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Dato' Seri. Dr. S. Sharavanan
President, VMRF

Dear Principal,

I'm happy the Vinayaka Mission Kirupananda Variyar Arts and Science College, Salem is organising "The 6th International e-Conference on Nanoscience and Nanotechnology for Energy, Environment and Biomedical Applications" (iNEEBA-2026) virtually on September 24-25, 2026.

I appreciate that this is the 6th edition of this flagship event, following three offline and two online conferences conducted during the previous years.

I hope this event will inspire more and more participants to take part in the deliberations and contribute towards a more sustainable and productive recommendations to improve the quality of healthcare practices for better living conditions.

I wish the conference a very big success.

Dato' Seri . Dr. S. Sharavanan



VINAYAKA MISSION'S RESEARCH FOUNDATION

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Hon'ble Dr. A. S. Ganesan
Chancellor
VMRF (DU)

It is a matter of great pleasure and pride to note that **Vinayaka Mission's Kirupananda Variyar Arts and Science College (VMKVASC)**, in association with **Gyeongsang National University**, South Korea, and **Chulalongkorn University**, Thailand, is organizing the **6th Indo–South Korea–Thailand International Conference on Nanoscience and Nanotechnology for Energy, Environment, and Biomedical Applications (iNEEBA-2026)** on **24–25 September 2026** through online mode.

The successful journey of **iNEEBA 2021–2025** is a testament to the dedication of the organizing team and the strong international academic collaborations established through this conference series. The continuation of iNEEBA reflects the growing importance of nanoscience and nanotechnology in addressing contemporary challenges in energy, environment, and biomedical sciences. This international conference provides an excellent opportunity for scientists, researchers, academicians, scholars, and students to exchange knowledge, present their research findings, and explore new avenues for interdisciplinary and international collaboration. It is a matter of immense pride that all five editions of **iNEEBA** have successfully showcased and facilitated the publication of high-quality research in **Scopus-indexed journals**, including the **IOP Journal of Physics: Conference Series** and **Applied Physics A**. It is truly encouraging to see that, this year too, the organising team has made dedicated efforts to provide avenues for publication in reputed Scopus-indexed journals. I sincerely commend the team for their continued commitment to fostering quality research and academic excellence through iNEEBA. This continued commitment towards quality research, international collaboration, and scholarly publication has significantly strengthened the academic stature and research impact of iNEEBA. I sincerely appreciate the efforts of the organizing committee and the collaborating institutions from India, South Korea, and Thailand in bringing together this valuable scientific platform. I wish **iNEEBA-2026** a grand success and hope that the conference will inspire meaningful research collaborations and contribute to the advancement of science and technology.

Hon'ble Dr. A. S. Ganesan



Mr. N.V. Chandrasekar
Vice President
VMRF (DU)

I am delighted to know that Vinayaka Mission's Kirupananda Variyar Arts and Science College (VMKVASC), in association with Gyeongsang National University, South Korea, and Chulalongkorn University, Thailand, is organizing the **6th Indo-South Korea-Thailand International Conference on Nanoscience and Nanotechnology for Energy, Environment, and Biomedical Applications (iNEEBA-2026)** on **24–25 September 2026** through online mode.

It is indeed gratifying to see the continued growth of the iNEEBA conference series following the remarkable success of **iNEEBA 2021–2025**. Over the years, the conference has provided a valuable platform for researchers and experts from different parts of the world to exchange ideas, share scientific knowledge, and establish meaningful collaborations. I am delighted to note that, over its five editions, **iNEEBA** has consistently provided a platform for high-quality research to reach reputed **Scopus-indexed journals**, including the **IOP Journal of Physics: Conference Series** and **Applied Physics A**. It is truly encouraging that the organising team has once again taken commendable initiatives to facilitate the publication of quality research in **Scopus-indexed journals** this year. I sincerely appreciate their sustained efforts and dedication towards promoting research excellence and further enhancing the academic stature of **iNEEBA**. **iNEEBA-2026** will provide an excellent forum to discuss recent advances, emerging technologies, challenges, and future directions in these multidisciplinary areas. I appreciate the commitment and tireless efforts of the organizing committee and the collaborating institutions. I am confident that this conference will be a rewarding experience for all participants.

I wish **iNEEBA-2026** every success.

Mr. N.V. Chandrasekar



Prof. Dr. P. K. Sudhir
Vice Chancellor
VMRF(DU)

It gives me immense pleasure to contribute this message to the **6th Indo–South Korea–Thailand International Conference on Nanoscience and Nanotechnology for Energy, Environment, and Biomedical Applications (iNEEBA-2026)**, organized by **Vinayaka Mission's Kirupananda Variyar Arts and Science College (VMKVASC)** in association with **Gyeongsang National University, South Korea, and Chulalongkorn University, Thailand**, on **24–25 September 2026 through online mode**. Nanotechnology continues to open new possibilities across diverse scientific disciplines. Its applications in sustainable energy, environmental remediation, advanced materials, and biomedical sciences are particularly significant in addressing the needs of modern society. I am also pleased to acknowledge that, through its five successful editions, **iNEEBA** has established a strong record of promoting impactful research and enabling its dissemination through reputed **Scopus-indexed journals**, including the **IOP Journal of Physics: Conference Series** and **Applied Physics A**. It is commendable that the organising team continues this tradition by creating valuable opportunities for scholarly publication this year as well. I sincerely congratulate the team for their unwavering commitment to advancing research, fostering scholarly collaboration, and elevating the academic impact of **iNEEBA**.

I am confident that **iNEEBA-2026** will facilitate the exchange of innovative ideas, encourage interdisciplinary collaborations, and provide young researchers with opportunities to interact with experts from India and abroad. I congratulate the organizing committee and extend my best wishes to all the invited speakers, presenters, researchers, and participants.

I wish **iNEEBA-2026** a highly successful and enriching conference.

Prof. Dr. P. K. Sudhir



VINAYAKA MISSION'S RESEARCH FOUNDATION

(Deemed to be University under section 3 of the UGC Act 1956)



Prof. Dr. J. Sabarinathan

Pro - Vice Chancellor

VMRF(DU)

It is with great pleasure that I note that Vinayaka Mission's Kirupananda Variyar Arts and Science College (VMKVASC), in collaboration with Gyeongsang National University, South Korea, and Chulalongkorn University, Thailand, is hosting the 6th Indo-South Korea-Thailand International Conference on Nanoscience and Nanotechnology for Energy, Environment, and Biomedical Applications (iNEEBA-2026) on 24–25 September 2026 through online mode.

The successful conduct of iNEEBA 2021–2025 stands as a testimony to the sustained efforts towards fostering international academic cooperation and promoting excellence in research and innovation. Over the years, the conference has evolved into a meaningful platform for scientific exchange, bringing together researchers and experts working across diverse domains of nanoscience and nanotechnology. The successful journey of the five editions of iNEEBA reflects its significant contribution to the research community, with noteworthy scientific contributions finding their way into prestigious **Scopus-indexed journals**, including the **IOP Journal of Physics: Conference Series** and **Applied Physics A**. The continued initiative to provide publication opportunities through this year's conference reflects the organising team's strong commitment to nurturing a culture of research and scholarly dissemination. I extend my sincere appreciation to the entire team for their sustained dedication to fostering meaningful collaborations and enhancing the academic and research prominence of **iNEEBA**.

iNEEBA-2026 provides an excellent forum for scientists, academicians, research scholars, students, and industry professionals to present their latest findings, exchange perspectives, and explore emerging opportunities in energy, environmental sustainability, and biomedical applications of nanotechnology. The online platform of this conference will further broaden its reach by enabling participation from researchers and experts across different regions of the world. I extend my best wishes for the grand success of iNEEBA-2026 and hope that the conference will pave the way for many fruitful collaborations and significant advancements in nanoscience and nanotechnology.

Prof. Dr. J. Sabarinathan



VINAYAKA MISSION'S RESEARCH FOUNDATION

(Deemed to be University under section 3 of the UGC Act 1956)



Prof. Dr. A. Nagappan

Registrar

VMRF(DU)

It gives me immense pleasure to send my warm compliments and best wishes on the occasion of the **6th Indo–South Korea–Thailand International Conference on Nanoscience and Nanotechnology for Energy, Environment, and Biomedical Applications (iNEEBA-2026)**, being organized by Vinayaka Mission's Kirupananda Variyar Arts and Science College (VMKVASC) in partnership with Gyeongsang National University, South Korea, and Chulalongkorn University, Thailand, **on 24–25 September 2026 through online mode.**

Nanoscience and nanotechnology stand today at the frontier of scientific innovation, offering transformative solutions to some of humanity's most pressing challenges in energy sustainability, environmental protection, and biomedical advancement. It is heartening to see iNEEBA continuing to serve as a meaningful bridge connecting researchers, academicians, and students across India, South Korea, and Thailand, a true testament to the power of international academic partnership in advancing science for the collective good.

Since its inception, iNEEBA has grown steadily in stature, earning recognition as a credible platform for quality research dissemination, with outcomes from previous editions finding their way into respected Scopus-indexed publications such as the IOP Journal of Physics: Conference Series and Applied Physics A. This is a reflection not merely of organizational diligence, but of a genuine and sustained commitment to nurturing research excellence and providing scholars a meaningful avenue to contribute to the global scientific discourse. I take this opportunity to compliment the organizing committee for upholding this tradition in the sixth edition as well.

The theme chosen for this year's conference, spanning **Energy, Environment, and Biomedical Applications** — could not be more relevant to the challenges and aspirations of our times. I am confident that the deliberations, presentations, and exchanges over the two days will yield valuable insights and open new avenues for collaborative research.

I convey my sincere appreciation to the organizing committee, coordinators, international partner institutions, keynote and invited speakers, reviewers, and all others whose dedication has made this conference possible.

To every delegate, researcher, scholar, and student participating in iNEEBA-2026, I extend my warmest wishes for a stimulating and productive conference.

May this conference continue to inspire scientific curiosity, foster meaningful collaborations, and contribute to a better and more sustainable future.

Prof. Dr. A. Nagappan



Dr. K. Manivannan
COE, VMRF(DU)

It is a great pleasure to acknowledge the remarkable progress of **Vinayaka Mission's Kirupananda Variyar Arts and Science College (VMKVASC)**, in association with **Gyeongsang National University, South Korea, and Chulalongkorn University, Thailand**, is organizing the **6th Indo-South Korea-Thailand International Conference on Nanoscience and Nanotechnology for Energy, Environment, and Biomedical Applications (iNEEBA-2026)** on **24–25 September 2026 in online mode**.

The remarkable journey and continued success of **iNEEBA 2021–2025** stand as a testament to the institution's steadfast commitment to **academic excellence, research innovation, and meaningful international collaboration**. Over its five editions, **iNEEBA** has emerged as a robust platform for the presentation, dissemination, and translation of cutting-edge research in **nanoscience and nanotechnology**, with significant research outcomes progressing to publication in reputed **Scopus-indexed journals**, including the **IOP Journal of Physics: Conference Series** and **Applied Physics A**. The continued emphasis on **peer-reviewed scholarly publication** in the present edition reflects the organising team's commitment to advancing scientific rigor, promoting interdisciplinary research, facilitating knowledge transfer, and strengthening international research networks. I sincerely appreciate the entire team for their sustained efforts in enhancing the **scientific impact, research visibility, collaborative potential, and global academic standing of iNEEBA**.

With its multidisciplinary focus on **energy, environment, and biomedical applications**, **iNEEBA-2026** provides an excellent platform for fostering intellectual exchange, interdisciplinary dialogue, and new avenues for research collaboration. The online mode of the conference further broadens its reach, enabling experts, researchers, and young scholars from across the world to participate and contribute to this global scientific dialogue.

I extend my sincere appreciation and congratulations to the **organizing committee and all those involved in making this international conference a success**. I wish every participant a **stimulating, productive, and enriching scientific experience**, and hope that the deliberations of **iNEEBA-2026** will inspire new ideas, strengthen collaborations, and contribute meaningfully to the advancement of science and technology.

I wish **iNEEBA-2026** great success.



Dr. K. Manivannan



VINAYAKA MISSION'S RESEARCH FOUNDATION

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Prof. Myong Yong Choi

Director of Core-Facility Center for
Photochemistry and Nanomaterials
Gyeongsang National University
Jinju, South Korea

It is a great pleasure to be associated with the **6th Indo–South Korea–Thailand International Conference on Nanoscience and Nanotechnology for Energy, Environment, and Biomedical Applications (iNEEBA-2026)**, organized by **Vinayaka Mission's Kirupananda Variyar Arts and Science College (VMKVASC)** in association with **Gyeongsang National University, South Korea, and Chulalongkorn University, Thailand**, on **24–25 September 2026 through online mode**.

The continued success of **iNEEBA 2021–2025** demonstrates the strong interest and commitment of researchers from different countries towards scientific exchange and international collaboration in nanoscience and nanotechnology. Over its five editions, **iNEEBA** has emerged as a distinguished platform for cutting-edge research in **nanoscience and nanotechnology**, with impactful research outcomes published in reputed **Scopus-indexed journals**, including the **IOP Journal of Physics: Conference Series** and **Applied Physics A**.

The continued focus on **peer-reviewed publication, interdisciplinary collaboration, knowledge transfer, and international research networking** reflects the organising team's commitment to scientific excellence and enhancing the global academic impact of **iNEEBA**. International collaboration between India, South Korea, and Thailand provides a valuable opportunity to strengthen scientific relationships and encourage future joint research activities. I am confident that **iNEEBA-2026** will generate meaningful discussions and open new avenues for collaboration. I sincerely appreciate the organizing committee for their continuous efforts and dedication. I wish all the participants a successful and rewarding conference.

Prof. Myong Yong Choi



Prof. Soorathep Kheawhom

Department of Chemical Engineering

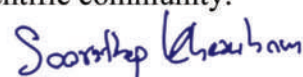
Faculty of Engineering

Chulalongkorn University, Thailand

It is a great honour and pleasure for me to be associated with the 6th Indo–South Korea–Thailand International Conference on Nanoscience and Nanotechnology for Energy, Environment, and Biomedical Applications (iNEEBA-2026), organized by Vinayaka Mission's Kirupananda Variyar Arts and Science College (VMKVASC) in collaboration with Gyeongsang National University, South Korea, and Chulalongkorn University, Thailand, on 24–25 September 2026 through online mode.

The remarkable journey of iNEEBA 2021–2025 reflects the sustained commitment of the participating institutions towards promoting scientific excellence, knowledge sharing, and international academic collaboration. Across its five editions, **iNEEBA** has promoted impactful research in **nanoscience and nanotechnology**, with quality contributions published in reputed **Scopus-indexed journals**, including **IOP Journal of Physics: Conference Series** and **Applied Physics A**. The continued publication initiatives this year reflect the organising team's commitment to **scientific excellence, interdisciplinary collaboration, and global research visibility**. iNEEBA-2026 provides an excellent opportunity to present recent discoveries, exchange innovative perspectives, and discuss emerging trends that can shape the future of nanoscience and nanotechnology.

I sincerely appreciate the efforts of the organizing committee, collaborating institutions, invited speakers, researchers, and all participants whose collective contributions have made iNEEBA a vibrant international scientific forum. I am confident that the deliberations and interactions at iNEEBA-2026 will generate new ideas, strengthen global research networks, and inspire innovative solutions for the benefit of society. I extend my heartfelt congratulations to the organizers and wish iNEEBA-2026 great success. I hope this international conference will be an intellectually enriching and inspiring experience for all participants and will pave the way for new discoveries, enduring collaborations, and a stronger global scientific community.



Prof. Soorathep Kheawhom

Message from the Organizing Committee

As the **Organizing Committee of iNEEBA-2026**, we are delighted to extend our warm greetings to all participants of the **6th Indo–South Korea–Thailand International Conference on Nanoscience and Nanotechnology for Energy, Environment, and Biomedical Applications**, organized by **Vinayaka Mission's Kirupananda Variyar Arts and Science College (VMKVASC)** in association with **Gyeongsang National University, South Korea, and Chulalongkorn University, Thailand**, on **24–25 September 2026 through online mode**.

It gives us immense pleasure to continue the successful journey of the iNEEBA conference series, which began in **2021** and has successfully brought together researchers, academicians, scientists, scholars, students, and industry professionals from different parts of the world. The remarkable response to **iNEEBA 2021–2025** has encouraged us to organize the sixth edition with renewed enthusiasm and commitment. As the **Organising Committee**, we take immense pride in the five successful editions of **iNEEBA**, which have promoted impactful research in **nanoscience and nanotechnology**, with quality contributions published in reputed **Scopus-indexed journals**, including the **IOP Journal of Physics: Conference Series** and **Applied Physics A**. We are equally pleased to continue this publication initiative this year, reflecting our commitment to **scientific excellence, interdisciplinary collaboration, and enhanced global research visibility**. iNEEBA-2026 is designed as a vibrant international forum for sharing **innovative ideas, recent research findings, emerging trends, technological developments, and future perspectives** in nanoscience and nanotechnology, with particular emphasis on energy, environment, and biomedical applications. We sincerely thank our collaborating institutions, invited speakers, researchers, academicians, students, and participants for their valuable support. We also express our gratitude to everyone who has contributed to making this international scientific event possible.

We warmly welcome you all to **iNEEBA-2026** and look forward to an intellectually stimulating, collaborative, and memorable conference.

With warm regards,

Organizing Committee

iNEEBA-2026

VMKVASC, Salem, India

PROCEEDINGS OF iNEEBA-2026

September 24-25, 2026

Editors

Prof. Dr. Myong Yong Choi

Director of Core-Facility Center for Photochemistry and Nanomaterials,
Gyeongsang National University (GNU),
South Korea

Prof. Dr. Soorathep Kheawhom

Professor of Chemical Engineering
Chulalongkorn University, Thailand

Dr. V. Anbazhagan

Professor & Principal
Vinayaka Mission's Kirupananda Variyar Arts and Science College
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**6th International e-Conference on Nanoscience and Nanotechnology for Energy,
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ISBN No.: 978-93-344-8849-4

Published by Vinayaka Mission's Kirupananda Variyar Arts and Science College
(A Constituent College of Vinayaka Mission's Research Foundation), Salem-636308,
Tamil Nadu, India



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Cordially invites you to

**Indo - South Korea – Thailand 6th International e-Conference on
Nanoscience and Nanotechnology for Energy, Environment and Biomedical
Applications (iNEEBA-2026)**

(ONLINE MODE) [24-25 September 2026]

In Collaboration with



PROGRAM SCHEDULE

DAY 1 | 24 SEPTEMBER 2026 | INAUGURAL FUNCTION | 10:00 AM-11:20 AM

INAUGURAL FUNCTION

Zoom Link:

<https://us06web.zoom.us/j/81883279490?pwd=VWmprNpFYDyYPxJaBTz73iqDdwWPKN.1>

Meeting ID: 818 8327 9490; Passcode: 662778

TIME	EVENT / PROGRAM	DIGNITARY / SPEAKER DETAILS
10.00 AM – 10.05 AM	Welcome Address	Prof. Dr. V. Anbazhagan Principal, VMKVASC, Salem, India
10.05 AM – 10.15 AM	Video Presentation	iNEEBA Milestones: A Journey of Success
10.15 AM – 10.25 AM	Inaugural Address	Prof. Dr. P.K. Sudhir Vice Chancellor, VMRFDU, Salem, India
10.25 AM – 10.35 AM	Pro-Vice Chancellor's Address	Prof. Dr. J. Sabarinathan Pro-Vice Chancellor, VMRFDU, Salem, India
10.35 AM – 10.45 AM	Registrar's Address	Prof. Dr. A. Nagappan Registrar, VMRFDU
10.45 AM – 11.00 AM	Special Address by Guest of Honor	Prof. Dr. Myong Yong Choi Director of Core-Facility Center for Photochemistry and Nanomaterials Gyeongsang National University (GNU), South Korea
11.00 AM – 11.15 AM	Presidential Address & Release of the Proceedings	Dr. A.S. Ganesan Chancellor, VMRFDU, Salem, India
11.15 AM – 11.20 AM	Vote of Thanks	Dr. J. Theerthagiri Research Professor – Brain Pool Fellow, Core-Facility Center for Photochemistry & Nanomaterials, Department of Chemistry, GNU, South Korea.

DAY 1 | 24 SEPTEMBER 2026 | TECHNICAL SESSIONS (DAY 1) | 11:30 AM–1:30 PM

Zoom Link:

<https://us06web.zoom.us/j/81883279490?pwd=VWmprNpFYDyYPxJaBTz73iqDdwWPKN.1>

Meeting ID: 818 8327 9490; Passcode: 662778

TIME	SESSION	SPEAKER & TOPIC DETAILS
11.30 AM – 12.00 PM	Keynote Lecture - I	Prof. Dr. Myong Yong Choi Director, Core-Facility Center for Photochemistry and Nanomaterials, GNU, South Korea Title: <i>Laser-Synthesized Electrocatalysts for Value-Added Chemical Production</i> Chairperson: Dr. V. Rajendiran, Associate Professor of Chemistry, Central University of Tamil Nadu, Thiruvavur, Tamil Nadu, India
12.00 PM – 12.30 PM	Invited Talk - I	Dr. Peng GAO Professor, Laboratory for Advanced Functional Materials (LAFM), Fujian Institute of Research on the Structure of Matter Chinese Academy of Science Jimei District, Xiamen P.R. China Title: <i>Suppressing Reverse-Bias Degradation and Deep-Level Defects in Perovskite Solar Cells via Molecular-Engineered Interfacial Layers</i> Chairperson: Prof. Dr. S. Manivannan, Professor of Physics, National Institute of Technology (NIT), Tiruchirappalli, Tamil Nadu, India
12.30 PM – 01.00 PM	Invited Talk - II	Prof. Dr. Anhar Abdel-Aziem Mohamed Professor of Organic Chemistry, Faculty of Science, Al-Azhar University, Cairo, Egypt Title: <i>Green Chemistry in Organic Synthesis: From Conventional to Sustainable Catalysts and Alternative Activation Methods</i> Chairperson: Prof. Dr. S. Mohana Roopan, Professor Department of Chemistry, School of Advanced Sciences (SAS), Vellore Institute of Technology (VIT), Vellore, Tamil Nadu, India
01.00 PM – 01.30 PM	Invited Talk - III	Dr. J. Theerthagiri Research Professor- Brain Pool Fellow, Core-Facility Center for Photochemistry & Nanomaterials, GNU, South Korea Title: <i>Laser-Enabled Design of Advanced Electrocatalysts for Sustainable Energy Technologies</i> Chairperson: Dr. M. Mohanraj, Associate Professor, Department of Chemistry, Dr. N.G.P. Arts and Science College, Coimbatore, Tamil Nadu, India
01.30 PM – 06.30 PM	PARALLEL SESSIONS	ORAL PRESENTATION & POSTER PRESENTATION

DAY 2 | 25 SEPTEMBER 2026 | TECHNICAL SESSIONS | 9:00 AM–11:40 AM

Zoom Link:

<https://us06web.zoom.us/j/81883279490?pwd=VWmprNpFYDyYPxJaBTz73iqDdwWPKN.1>

Meeting ID: 818 8327 9490; Passcode: 662778

TIME	SESSION	SPEAKER & TOPIC DETAILS
09.00 AM – 09.10 AM	Welcome & Recap of Day 1	Session Moderator
09.10 AM – 09.40 AM	Keynote Lecture - II	Dr. G. Arthanareeswaran, Senior Professor and Head, Department of Chemical Engineering, National Institute of Technology, Tiruchirappalli, India Title: Membrane Innovations: Materials and Technologies Shaping the future of Energy and Environment Chairperson: Dr. M. Saravanabhavan, Associate Professor, Department of Chemistry, KPR Institute of Engineering and Technology, Coimbatore, Tamil Nadu, India
09.40 AM – 10.10 AM	Invited Talk - I	Dr. V. Rajendiran, Associate Professor of Chemistry, School of Basic and Applied Sciences, Central University of Tamil Nadu, Thiruvarur, Tamil Nadu, India Title: <i>Copper(II) and Ruthenium(II) Complexes as Potential Anticancer Agents</i> Chairperson: Dr. Omkar Singh Kushwaha, Senior Principal Project Scientist, Department of Chemical Engineering, Indian Institute of Technology Madras (IIT Madras), Chennai, Tamil Nadu, India
10.10 AM – 10.40 AM	Invited Talk - II	Dr. Aruna Kumari M. L., Assistant Professor & Head, Department of Chemistry, The Oxford College of Science, Bangalore, India Title: <i>In Situ Spectroscopic Characterization of Energy Materials: Unveiling Dynamic Interfacial Mechanisms in Electrochemical Reactions</i> Chairperson: Dr. K. Manikandan, Assistant Professor, Department of Chemistry, SRM Institute of Science and Technology, Chennai, Tamil Nadu, India
10.40 AM – 11.10 AM	Invited Talk - III	Prof. S. Manivannan, Professor of Physics, National Institute of Technology (NIT), Tiruchirappalli, Tamil Nadu, India Title: <i>Pure and Doped Carbon Nanostructures for Energy Storage and Biomedical Sensing</i> Chairperson: Dr. M. Revathi, Associate Professor, Department of Chemistry, Vels Institute of Science, Technology and Advanced Studies, Chennai, Tamil Nadu, India
11.10 AM – 11.40 AM	Invited Talk - IV	Dr. Omid Sharifahmadian, Professor, Department of Coating Processes, FunGlass – Centre for Functional and Surface Functionalized Glass Alexander Dubček University of Trenčín, Slovakia Title: <i>Tailoring Diamond-Like Carbon (DLC) Coatings: Doping Strategies, Layer Architectures, and Multi-Functional Applications</i> Chairperson: Dr. Rajkumar Subramani, Assistant Professor of Chemistry, Central University of Tamil Nadu, Thiruvarur, Tamil Nadu, India
11.40 AM – 03.30 PM	PARALLEL SESSIONS	ORAL PRESENTATION & POSTER PRESENTATION

DAY 2 | 25 SEPTEMBER 2026 | VALEDICTORY FUNCTION [04.00 PM-5.00 PM]

Zoom Link:

<https://us06web.zoom.us/j/81883279490?pwd=VWmprNpFYDyYPxJaBTz73iqDdwWPKN.1>

Meeting ID: 818 8327 9490; Passcode: 662778

Time	Event / Program	Dignitary / Details
04.00 PM – 05.00 PM	Welcome Address	Prof. Dr. M. Prakash, VMKVASC, Salem
	Felicitation	Prof. Dr. S. Rajendran Co-Editor of Materials Protection St. Antony's College, Dindigul
	Conference Report	Dr. E. Shinyjoy, VMKVASC, Salem
	Valedictory Address & Presentation of Chancellor's Award & Young Scientist Award	Prof. Dr. A. Nagappan Registrar VMRF(DU), Salem
	Vote of Thanks	Dr. R. Ganesamoorthy, VMKVASC, Salem

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iNEEBA-2026 KEYNOTE LECTURE & INVITED TALK

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2	Suppressing Reverse-Bias Degradation and Deep-Level Defects in Perovskite Solar Cells via Molecular-Engineered Interfacial Layers Gao Peng	2
3	Green Chemistry in Organic Synthesis: From Conventional to Sustainable Catalysts and Alternative Activation Methods Anhar Abdel-Aziem	3
4	Laser-Enabled Design of Advanced Electrocatalysts for Sustainable Energy Technologies Theerthagiri Jayaraman	4
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Laser-Synthesized Electrocatalysts for Value-Added Chemical Production

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Abstract

The global energy crisis is increasing the demand for innovative materials with high purity and functionality for the development of clean energy production and storage. The development of novel photo- and electrocatalysts depends significantly on synthetic techniques that enable the production of tailored, advanced nanomaterials. The emerging use of pulsed laser in liquid synthesis has attracted immense interest as an effective synthetic technology with several advantages over conventional chemical and physical synthetic routes, including the fine-tuning of size, composition, surface, and crystalline structures, and defect densities, and is associated with the catalytic, electronic, thermal, optical, and mechanical properties of the produced nanomaterials. Herein, we present an overview of the fundamental understanding and importance of the pulsed laser process, namely, the various roles and mechanisms involved in the production of nanomaterials, including metal nanoparticles, oxides, non-oxides, and carbon-based materials. Herein, we mainly cover the advancement of photo- and electrocatalytic nanomaterials via pulsed laser-assisted technologies, with detailed mechanistic insights and structural optimization, along with effective catalytic performance in CO₂ conversion for value-added fuel and chemical production processes.

Suppressing Reverse-Bias Degradation and Deep-Level Defects in Perovskite Solar Cells via Molecular-Engineered Interfacial Layers

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Abstract

Interfacial reactions and deep-level defects are the primary causes of efficiency loss and operational-stability degradation in perovskite solar cells (PSCs). This report presents our group's progress in the molecular engineering of interfacial layers: (1) To address the chemical degradation at the NiOx/perovskite interface under reverse bias, we designed an o-SAM interfacial layer that suppresses the Ni³⁺ reduction reaction; the resulting device remained stable after −1 V treatment for 6 h (efficiency 24.2%). (2) We quantitatively identified the dominant role of IFA and IPb deep-level defects in degradation, and proposed a non-intercalating 3TU ligand passivation strategy that eliminates the early rapid decay, achieving a certified efficiency of 25.6%, a T80 lifetime exceeding 10 years, and a levelized cost of electricity of 0.148 USD/kWh. (3) Combined with the long-term outdoor demonstration of a 2 kW perovskite module in Xiamen, we elucidated its power-generation behavior under seasonal and extreme-weather conditions, as well as its advantages over silicon cells under high-temperature and low-light conditions, and identified outdoor-stability bottlenecks such as edge degradation and hot spots. These results provide new insights for the interfacial design of long-lifetime perovskite photovoltaic devices.

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Green Chemistry in Organic Synthesis: From Conventional to Sustainable Catalysts and Alternative Activation Methods

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Abstract

Conventional organic synthesis often relies on hazardous reagents and solvents, generates significant chemical waste, requires high energy input, and may involve prolonged reaction times and harsh reaction conditions. These practices can have significant environmental impacts, highlighting the need for more sustainable approaches to organic synthesis. Green chemistry provides a powerful framework for designing chemical processes that minimize waste, reduce hazardous substances, improve energy efficiency, and promote the use of safer and renewable resources. This lecture presents an overview of the transition from conventional to greener organic synthesis, with particular emphasis on sustainable catalytic systems and alternative activation methods. Key strategies including the use of lemon juice as natural catalysts, microwave irradiation, ultrasound-assisted synthesis, and mechanochemical/grinding techniques will be discussed as effective approaches for improving reaction efficiency while reducing environmental impact. Selected examples of the synthesized heterocyclic compounds from our research on environmentally friendly organic synthesis will be presented to demonstrate how green catalytic systems and alternative activation techniques can lead to simpler, cleaner, and more energy-efficient synthetic processes.

Laser-Enabled Design of Advanced Electrocatalysts for Sustainable Energy Technologies

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Abstract

The global energy crisis is driving an increasing demand for innovative materials with high purity and functionality to enable the development of clean energy production and storage solutions. The advancement of novel photo- and electrocatalysts heavily relies on synthetic techniques that support the creation of tailored advanced nanomaterials. The emerging application of pulsed lasers in liquid synthesis has garnered significant attention as an effective synthetic technology, offering numerous advantages over conventional chemical and physical synthesis methods. This study primarily focuses on the advancements in electrocatalytic nanomaterials achieved through pulsed laser-assisted technologies, providing detailed mechanistic insights, structural optimization, and demonstrating their effective catalytic performance in hydrogen fuel production and the generation of value-added chemicals.

Copper (II) and Ruthenium (II) Complexes as Potential Anticancer Agents

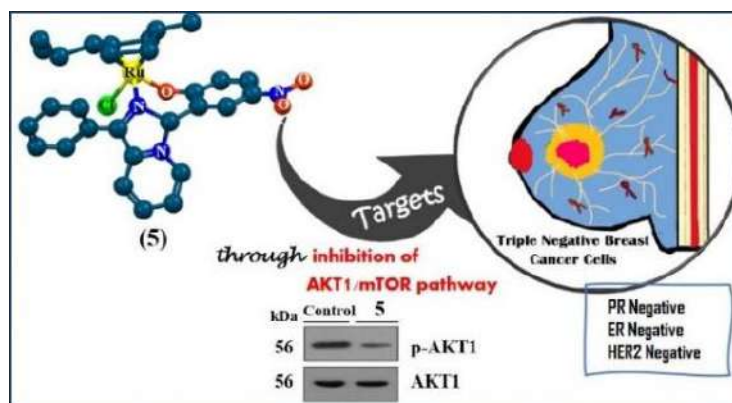
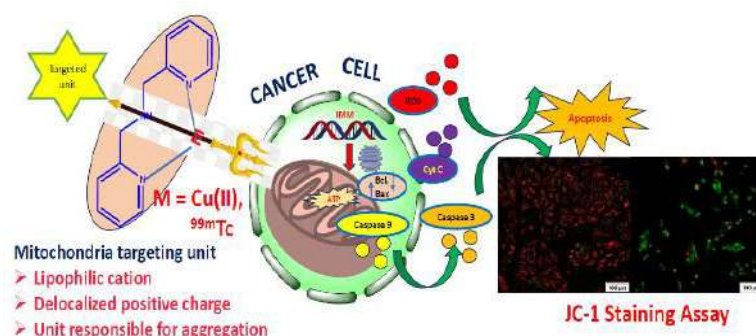
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Abstract

Cancer is a primary global mortality factor, prompting heightened interest in designing safer anticancer therapeutics. Although many organic molecules are in clinical use, metal-based drug design has received much attention among medicinal chemists since the FDA approved cisplatin for a few cancer types. However, it faces issues of cellular resistance and significant side effects, creating room for designing metal-based drugs as an alternative to cisplatin. Among transition-metal complexes, copper- and ruthenium-based complexes can serve as alternatives to platinum-based drugs for the following biological applications. Copper(II) complexes can be the most promising candidates, as they are endogenous trace elements deeply involved in redox control, angiogenesis, and mitochondrial function in cancer cells. Copper(II) complexes exhibit multifaceted cytotoxicity: their redox cycling (Cu(II)/Cu(I)) generates reactive oxygen species (ROS), depletes glutathione, and disrupts DNA/protein integrity. Hence, the development of copper-based chemotherapeutics has received considerable attention from medicinal chemists. Like copper, ruthenium(III/II) complexes are equally crucial in designing new metal-based drugs, and a few of them have entered clinical trials. Ruthenium possesses advantageous chemical properties, including versatile photophysical and redox properties (Ru^{II} and Ru^{III}). Moreover, ruthenium complexes exhibit fewer side effects than platinum-based anticancer agents, possibly because they can reach the cancer site via the transferrin-mediated pathway. Hence, we hypothesized that the design and synthesis of copper(II) and ruthenium(II) complexes by varying the ligand frame and tuning their properties toward the tumor microenvironment would pave the way for the development of promising metal-based anticancer agents. In the present investigation, we prepared a series of copper(II) and ruthenium(II) complexes, systematically characterized them, tested their in vitro cytotoxicity and mechanism of cell-death. Finally, evaluated their structure-activity relationship. In light of the above, we identified a few of them that could be developed into promising anticancer agents. All the results will be discussed systematically.



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In Situ Spectroscopic Characterization of Energy Materials: Unveiling Dynamic Interfacial Mechanisms in Electrochemical Reactions

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Abstract

Evaluating the real-time structural evolution and phase transformations of energy materials during electrochemical energy reactions is foundational to developing next-generation energy conversion and storage technologies. Traditional ex situ techniques fail to capture the transient intermediates, surface rearrangements, and highly dynamic redox states that dictate catalytic activity and degradation pathways under operational conditions. Herein provides a comprehensive, comparative analysis of recent advancements, engineering paradigms, and boundary constraints in in-situ and operando Raman, Fourier-transform infrared (FTIR), and X-ray photoelectron spectroscopy (XPS). For in situ Raman spectroscopy, we address the mitigation of background fluorescence, the elimination of spectral overlap from common electrode substrates, and the utilization of advanced plasmonic configurations—including tip-enhanced, surface-enhanced, and shell-isolated nanoparticle-enhanced variants—that dramatically amplify weak vibrational signals to enable the detection of trace intermediate species at the interface. Turning to in situ FT-IR spectroscopy, the critical trade-off between signal attenuation and mass transport across internal and external reflection configurations, examining how potential modulation and subtractive normalization techniques map electrochemical sequences to discrete molecular vibrations through chemically resistant, broadband crystals. Finally, the environmental and pressure constraints of in situ XPS by analyzing how short electron path lengths are managed via advanced spectroelectrochemical cell configurations, including thin-film liquid layers, protective microcell membranes, and ambient pressure environments paired with specialized electrolytes. By leveraging advanced synchrotron radiation and high-flux X-ray sources, these combined toolsets reveal true chemical states, oxidation gradients, and structural deactivation pathways under realistic operational conditions, establishing a clear methodology for pairing complementary vibrational and electronic characterization to accelerate the design of high-performance energy materials.

Pure and Doped Carbon Nanostructures for Energy Storage and Biomedical Sensing

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Abstract

Carbon nanomaterials, including graphene oxide (GO), reduced graphene oxide (rGO), carbon nanotubes (CNTs), and carbon dots (CDs), have emerged as versatile platforms bridging energy, environment and healthcare technologies, owing to their tunable electronic, optical and surface properties. Lattice irregularities, cross hybridization, localized geometries, sp^2 and sp^3 structural puckering, provide strategies for tailoring pristine and heteroatom-doped (N, B, P, S, Br, etc.) carbon architectures to enhance performance across the domains. For instance, in energy storage, heteroatom doping of GO/rGO significantly improves charge carrier density and porosity, yielding high specific capacitances and asymmetric supercapacitors delivering energy densities (>40 Wh/kg) validated through practical demonstrations such as LED illumination and motor operation. In biomedical and environmental sensing, biomass and precursor-derived carbon dots doped with N, P, and other heteroatoms act as fluorescence-based ratiometric sensors for Fe^{3+} , hippuric acid, and glutathione, with detection limits in the nanomolar-to-micromolar range and validated performance in real biological samples (tap water, urine). Together, these results demonstrate that structural engineering of carbon nanomaterials via controlled doping offer a unifying design principle for next-generation, cost-effective devices spanning clean energy storage and point-of-care bio-sensing without distressing the environment.

Tailoring Diamond-Like Carbon (DLC) Coatings: Doping Strategies, Layer Architectures and Multi-Functional Applications

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Abstract

Diamond-like carbon (DLC) thin films offer exceptional hardness and low friction, yet their industrial adoption remains limited by high residual compressive stress, poor substrate adhesion, and environmental sensitivity. This presentation provides a comprehensive perspective on overcoming these mechanical and tribological issues through elemental doping, architectural design, and advanced plasma processing. The fundamental mechanisms by which non-metallic dopants alter the carbon networks sp^2/sp^3 bonding ratio, relax intrinsic strain, and tailor surface energy are established. Plasma process optimization strategies are examined, highlighting achievements in wear mitigation, corrosion protection, and hydrophobic surface functionality. Additionally, interface engineering through functionally graded multilayer structures is evaluated as a design approach to dissipate interfacial stress, suppress crack propagation, and enhance critical load-bearing capacity. Combined, these chemical and structural modification techniques provide a versatile, scalable framework for designing customized DLC coatings suitable for demanding industrial, optical, and biomedical applications.

Key Words: Carbon, Plasma, Multilayer, Tribology, Hydrophobicity, Interfacial Adhesion.

Targeted d-Orbital Modulation via Lanthanum Pillaring Delivers Phase-Stable δ -MnO₂ for Advanced Ammonium-Ion Storage

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Abstract

Aqueous ammonium-ion (NH₄⁺) storage has emerged as a promising alternative to metal-ion systems because NH₄⁺ combines a low molar mass with favorable transport kinetics. However, cooperative Jahn–Teller distortion, sluggish ion transport, and Mn dissolution limit the reversibility of layered MnO₂ cathodes. Here, we report La/NH₄⁺-co-intercalated δ -MnO₂ (LAMO), prepared via ultrafast CO₂-laser-assisted synthesis and subsequent ion exchange, to regulate both the electronic structure and interlayer chemistry of δ -MnO₂. La³⁺ pillaring increases the Mn⁴⁺ population, suppresses cooperative Jahn–Teller distortion, and stabilizes the MnO₆ octahedra, whereas NH₄⁺ establishes dynamic N–H $\cdots$ O hydrogen-bond networks that enable low-barrier twist-and-rotate transport. LAMO delivers a specific charge of 252 C g^{−1} at 0.5 A g^{−1} and retains approximately 90% of its capacity after 2000 cycles at 1 A g^{−1}. *In situ* Raman spectroscopy and *ex situ* XRD, XPS, and TOF-SIMS support a reversible, solid-solution-like NH₄⁺ storage mechanism accompanied by symmetric lattice breathing. Density functional theory calculations further indicate La-induced electronic delocalization, strengthened Mn–O interactions, and a reduced NH₄⁺ migration barrier of 0.31 eV. These findings identify coupled electronic and interlayer engineering as an effective strategy to stabilize layered oxides for fast, durable ammonium-ion storage.

Ru Single-atom Co₃O₄Nanosheet Catalyst for C1/C2 Simultaneous Production PET Upcycling

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Abstract

The electrochemical oxidation of biomass-derived ethylene glycol (EG) offers a promising route for upcycling into high-value chemicals; however, achieving the selective co-production of specific C1 and C2 products remains a significant challenge. Here, we report a ruthenium single-atom catalyst anchored on cobalt oxide nanosheets (RuSA/Co₃O₄) designed for the highly efficient and simultaneous synthesis of formate (C1) and glycolate (C2) via the ethylene glycol oxidation reaction (EGOR). Comprehensive structural and chemical characterizations using XRD, HAADF-STEM, and XAS confirm the atomic dispersion of Ru active sites and strong metal-support interactions (SMSI) with the Co₃O₄ matrix. Electrochemical analyses reveal that this unique atomic configuration effectively regulates the surface adsorption energies of key intermediates, establishing a delicate balance between partial C-C bond cleavage and selective C2 retention. Consequently, the optimized RuSA/Co₃O₄ catalyst demonstrates superior catalytic activity, high overall Faradaic efficiency for both formate and glycolate, and exceptional long-term durability. This study presents a practical catalyst design strategy for controlling C-C bond cleavage dynamics, paving the way for the economical, multi-product electrosynthesis of complex polyols.

Keywords: Ethylene glycol oxidation reaction; single atom catalysis; Co₃O₄ nanosheets; PET upcycling

NiCuPd Medium-Entropy Alloy by Pulsed-Laser-Engineering Electrocatalyst for Efficient Glycerol Electro Oxidation Reaction

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Abstract

The rapid growth of biodiesel production has generated substantial quantities of glycerol as a low-value byproduct, motivating the development of efficient routes for its conversion into value-added chemicals. Electrochemical glycerol oxidation offers an attractive approach, but the complex and competing reaction pathways make selective production of targeted oxidation products challenging. Herein, we report an equimolar NiCuPd medium-entropy alloy (MEA) synthesized by pulsed-laser irradiation in liquid (PLIL) as an efficient electrocatalyst for the glycerol oxidation reaction (GOR). The rapid and highly nonequilibrium conditions generated by PLIL promote the formation of a single-phase face-centered-cubic NiCuPd alloy with a homogeneous multimetallic structure. Incorporation of Ni and Cu into the Pd framework induces substantial interfacial charge redistribution and modulates the electronic structure of the alloy, thereby regulating the adsorption and conversion of glycerol-derived intermediates. These electronic interactions regulate the adsorption and conversion of glycerol-derived intermediates, thereby promoting GOR kinetics and favoring the formation of value-added chemical. This work highlights medium-entropy alloy engineering as an effective approach for directing glycerol electrooxidation toward value-added products.

Keywords: Pulsed-laser synthesis; NiCuPd medium entropy alloy; Electrocatalyst; Glycerol oxidation reaction; Value-added chemical production

Fe Single-Atom Sites Anchored on CuRu Nanowires via Rapid CO₂ Laser Synthesis for High Ammonia and Energy Generation

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Abstract

The electrochemical nitrate reduction reaction (NO₃RR) to ammonia is hindered by competing hydrogen evolution reaction (HER), complex multi-electron transfer pathways, and sluggish kinetics. Herein, we present a highly efficient strategy for selective NO₃RR to ammonia using Fe single atoms stabilized on tryptophan-modified CuRu nanowires (Fe SACs/Try-CuRu NWs) electrocatalyst. Atomically dispersed Fe single-atomic sites were constructed on a bimetallic CuRu nanowire support via a rapid CO₂ laser-induced synthesis, utilizing N-containing functional groups of tryptophan for assisted coordination. This approach offers a non-equilibrium and time-efficient route beyond conventional single-atom catalyst synthesis. Within this synergistic architecture, Fe sites act as key centers for NO₃⁻ activation, Cu facilitates intermediate conversion, and Ru enhances hydrogenation kinetics. The Fe SACs/Try-CuRu NWs catalyst achieved an outstanding Faradaic efficiency (FE) of 94.49% for NO₃RR at -0.6 V vs. RHE. Furthermore, in situ Raman spectroscopy and ex situ FT-IR confirmed the reaction pathways and provided profound insights into the enhanced NO₃RR performance. Integration of Fe SACs/Try-CuRu NWs into a Zn–nitrate battery further enables a dual-functional system for simultaneous ammonia production and electricity generation. This work highlights the potential of rapid laser technology and synergistic bimetallic engineering for the design of single-atom–stabilized nanostructures for sustainable energy conversion and environmental applications.

Lattice–Surface Dual-Site Engineering of Pd–Pt Dimers for Cascade Formamide Electrosynthesis

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Abstract

Electrocatalytic C–N coupling offers a sustainable route for organonitrogen compound synthesis under ambient conditions, yet formamide electrosynthesis remains constrained by sluggish oxidation kinetics and limited understanding of reaction pathways. Herein, we report an asymmetric heterodimer catalyst contain lattice-coordinated Pd and surface-coordinated Pt anchored on conductive Ti₃C₂T_xMXene for electrooxidative formamide synthesis via coupling of ethylene glycol and NH₄OH. The catalyst delivers a high formamide production rate of 133.2 mmol h^{−1}cm^{−2} under ambient conditions, attributed to accelerated interfacial charge transfer and lowered activation barriers. Mechanistic lattice-coordinated Pd sites act as carbon-activation sites for C–C, C–H bond cleavage and formyl stabilization, while surface-coordinated Pt sites serve as nitrogen activation centers substantially enabling C–N bond formation. The simultaneous evolution of aldehydic C–H, carbonyl, and N–H vibrational signatures identifies a sequential aldehyde → formyl → formamide pathway through tandem surface-mediated coupling. This cascade is accelerated by the dynamic generation of Ti–OOH/Ti–OO[−] active oxygen species that facilitate proton-coupled electron transfer and sustain the oxidative dehydrogenation microenvironment. This work provides a mechanistically resolved strategy for the ambient upcycling of waste-derived alcohols via atomically dispersed anodic dual sites.

Key words: Lattice-coordinated metal sites; Surface-coordinated metal sites; Asymmetric Pd–Pt Dimer; Formamide electrosynthesis; Heteroatomic dimer catalysis

Surface-Stabilized Pd Sites Modulate NiFe-LDH Hollow Nanocages for Selective Glycerol-to-Formate Electrosynthesis

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Abstract

Electrochemical glycerol oxidation provides an attractive route for converting an abundant biodiesel-derived byproduct into value-added chemicals, but directing the complex reaction network toward selective C1 products remains challenging. Herein, we report a Pd-site-engineered NiFe layered double hydroxide (Pd/NiFe-LDH) hollow nanocage catalyst for selective glycerol electrooxidation to formate. The MIL-88A-derived NiFe-LDH nanocages provide a highly accessible catalytic architecture, while rapid CO₂-laser treatment enables Pd incorporation within 5 min without compromising the hollow morphology. Pd-site integration modulates the electronic structure of the NiFe-LDH framework, as reflected by the enhanced Ni redox response, and facilitates glycerol oxidation. The optimized Pd/NiFe-LDH catalyst requires only 1.441 V versus the reversible hydrogen electrode to deliver 10 mA cm⁻² and achieves a formate Faradaic efficiency of 60% with a yield rate of 0.62 mmol h⁻¹ cm⁻². In situ Raman spectroscopy and electrochemical impedance measurements further reveal potential-dependent intermediate evolution and accelerated interfacial charge transfer during glycerol oxidation. These findings establish rapid laser-induced Pd-site engineering as a strategy for regulating the electronic structure and reaction pathways of LDH electrocatalysts and enable selective glycerol valorization to formate.

Pulsed-Laser-Driven Cu Engineering of Rock-Salt FeCoO for Paired Nitrate–Sulfide Electrolysis

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Abstract

In recent years, coupling the nitrate reduction reaction (NO₃RR) with the sulfide oxidation reaction (SOR) has emerged as a promising strategy for simultaneous pollutant remediation and value-added chemical co-production. The practical implementation of this system is hindered by several intrinsic challenges, including the competing hydrogen evolution reaction (HER) during the NO₃RR and the overoxidation of sulfide during SOR, both of which compromise product selectivity and process efficiency. Therefore, developing a bifunctional electrocatalyst capable of simultaneously regulating nitrate and sulfide reaction pathways remains highly desirable. Herein, we report a Cu incorporated FeCoO rock–salt catalyst fabricated via pulsed laser irradiation-thermal-assisted strategy. The incorporation of Cu effectively tailors the electronic structure of FeCoO and promotes the formation of catalytically active interfacial sites. As a result, the catalyst promotes selective sulfide oxidation, facilitating efficient conversion of polysulfide (S_x²⁻) generation. Simultaneously, under reduction conditions, the Cu–FeCoO catalyst undergoes in situ surface reconstruction, generating defect-rich active sites with optimized electronic configurations and abundant catalytic interfaces. The reconstructed catalyst exhibits NO₃RR performance, delivering a high ammonia (NH₃) Faradaic efficiency (FEs) of 92.16 % with a yield rate of 10.8 mg h⁻¹·cm⁻² at a reduction potential of -0.4 V versus reversible hydrogen electrode (RHE). When integrated into a NO₃RR||SOR electrolyzer, achieves efficient co-production of NH₃ and S_x²⁻ product with a low cell voltage of 1.5 V and remarkable operation stability exceeding 500 h.

Keywords: Pulsed laser irradiation; Cu–FeCoO catalyst; Electrocatalysis; NH₃ production; polysulfide production.

CuO Nanorods with Electronically Coupled Iridium Single Atoms for Highly Efficient and Stable Alkaline Water Oxidation

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Abstract

The oxygen evolution reaction (OER) is a key anodic process for electrochemical water splitting, yet its intrinsically sluggish kinetics impose substantial energy losses and motivate the development of highly active and durable electrocatalysts. Herein, we report ultrathin Ir-modified CuO nanorods with diameters of approximately 5–7 nm, synthesized through a pulsed-laser irradiation strategy. The rapid laser-mediated process enables the incorporation of Ir into the CuO framework while generating an ultrathin nanorod architecture, thereby modifying the local electronic structure and increasing the exposure of catalytically accessible sites. The resulting Ir–CuO catalyst exhibits markedly enhanced OER activity, requiring an overpotential of only 288 mV to deliver 10 mA cm^{−2}, outperforming commercial IrO₂ under identical alkaline conditions. The catalyst also retains its electrochemical activity during prolonged operation, indicating favorable structural and catalytic stability. The enhanced performance is attributed to the coupled effects of nanoscale structural engineering and Ir-induced electronic modulation of the CuO matrix. This work demonstrates pulsed-laser engineering as an effective strategy for tailoring oxide nanostructures and provides a route toward efficient and durable electrocatalysts for alkaline water oxidation.

Keywords: Pulsed-laser synthesis; Ir-modified CuO; Ultrathin nanorods; Electrocatalysis; Oxygen evolution reaction

CO₂ Laser-Driven Construction of K-hWO₃/Ti₃C₂T_x Heterostructures for High-Rate Aqueous Ammonium-Ion Storage

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Abstract

The development of electrode materials with rapid ion transport and structural stability is essential for aqueous ammonium-ion energy storage. Herein, for the first time, a CO₂ laser-enabled molten route was employed to synthesize K-intercalated hexagonal WO₃ (K-hWO₃) nanorods within only 2 min, followed by electrostatic assembly with Ti₃C₂T_xMXene to form a K-hWO₃/ Ti₃C₂T_x heterostructure nanocomposite. The heterostructure suppresses MXene restacking while facilitating rapid NH₄⁺ transport and electron transfer. Electrochemical analyses reveal dominant pseudocapacitive charge storage, with a capacitive contribution exceeding 61% at 5 mV s⁻¹, attributed to surface redox reactions at oxygen-terminated MXene sites and reversible NH₄⁺ insertion into K-hWO₃ tunnels. A full cell coupled with an NH₄V₃O₈ cathode operates stably over a 1.6 V window, delivering high energy and power densities while maintaining a Coulombic efficiency above 99% over 5000 cycles. These results demonstrate a rapid CO₂ laser-based strategy for constructing heterostructured electrodes and highlight K-hWO₃/ Ti₃C₂T_x as a promising material for high-performance aqueous ammonium-ion energy storage.

Cr-Induced Electronic Reconstruction of Laser-Engineered FeCo₂O₄ for Efficient Sulfide Oxidation-Coupled Hydrogen Production

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Abstract

Herein, we develop a Cr-induced electronically reconstructed FeCo₂O₄ electrocatalyst through a facile laser-engineering strategy for energy-efficient sulfide oxidation-coupled hydrogen production. The incorporation of Cr into the FeCo₂O₄ framework induces substantial electronic redistribution and modulates the local coordination environment, thereby generating catalytically favorable active sites for sulfide oxidation reaction (SOR). The optimized Cr–FeCo₂O₄ catalyst exhibits outstanding SOR activity, requiring only 0.41 V vs. RHE to achieve 50 mA cm⁻² for sulfide oxidation. Moreover, the catalyst promotes the selective conversion of sulfide species into valuable sulfur products, demonstrating its potential for simultaneous sulfide resource recovery and hydrogen generation. Benefiting from the accelerated reaction kinetics at both electrodes, the Pt/C(-)|| Cr-FeCo₂O₄-2(+) electrolyze achieves 50 mA cm⁻² at an ultralow cell voltage of 0.23 V, substantially outperforming conventional SOR||HER water electrolysis, which requires 1.85 V. Experimental characterizations and density functional theory calculations reveal that Cr incorporation triggers electronic reconstruction within the FeCo₂O₄ lattice, optimizing the electronic structure and adsorption characteristics of key SOR and HER intermediates. The resulting electronic modulation facilitates sulfide activation and sulfur formation at the anodic interface while promoting efficient water dissociation and hydrogen evolution at the cathode. This work establishes Cr-induced electronic reconstruction as an effective strategy for engineering laser-derived transition-metal oxides toward low-energy hydrogen production coupled with the valorization of sulfide resources.

Kinetics of Site-Selective Bond Activation on Ru-Pd/NiCo₂O₄ for Polyol Oxidation Reactions

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Abstract

Selective electrooxidation of biomass-derived polyols is limited by the coupled evolution of adsorption geometry, interfacial solvation and C–C bond cleavage as hydroxyl density increases. Here we report crystalline NiCo₂O₄ nanosheets bearing atomically dispersed PdRu dual sites as a kinetic platform for alcohol to polyol oxidation. Atomic-resolution microscopy and spectroscopy confirm that both Pd and Ru atoms are stabilized within the crystalline NiCo₂O₄ lattice, forming a dual-site interface on a redox-active spinel scaffold. Compared with NiCo₂O₄ and the corresponding Pd or Ru single-atom catalysts, PdRu-DSA/NiCo₂O₄ markedly enhances C–C cleavage selectivity and formate-generating polyol oxidation across ethylene glycol, glycerol, erythritol and xylitol. Temperature dependent electrochemical kinetics reveal that the dual-atom catalyst does not merely reduce the apparent activation energy, but reorganizes the entropy-enthalpy relationship governing polyol oxidation. As the hydroxyl density of the substrate increases, NiCo₂O₄ and single-atom catalysts show divergent kinetic responses, whereas PdRu-DSA/NiCo₂O₄ preserves a coherent Arrhenius trajectory with reduced substrate-dependent dispersion. These findings identify Pd–Ru dual single atom cooperativity as an interfacial pre-organization motif that couples multidentate polyol adsorption, hydroxide activation and C–C bond cleavage, offering a kinetic design rule for complex biomass electrooxidation.

Keywords: Electrocatalytic polyol oxidation; dual single atom catalysis; NiCo₂O₄ nanosheets; temperature-dependent kinetics; entropy-enthalpy compensation; C–H/C–C bond activation

Rapid CO₂ Laser Synthesis of Pt Single-Atom/rGO for Hydrazine-assisted Hydrogen Production

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Abstract

Overall water splitting (OWS) is a promising route for sustainable hydrogen production, but its efficiency is limited by the sluggish kinetics of the oxygen evolution reaction (OER) and its relatively high overpotential. Hydrazine oxidation reaction (HzOR) has emerged as an attractive alternative anodic reaction owing to its favorable thermodynamics and faster kinetics, offering a promising strategy for energy-efficient hydrogen production. Herein, we develop Pt single-atom (SA)-doped reduced graphene oxide (Pt SA/rGO) through an ultrafast CO₂ laser-assisted synthesis strategy. Graphene oxide (GO) was rapidly reduced to rGO within 40 s by CO₂ laser irradiation, followed by the incorporation of atomically dispersed Pt species within 5 min through a second laser treatment. This approach enables the rapid construction of a conductive, defect-rich rGO support with highly dispersed Pt active sites for efficient HzOR. The electrocatalytic performance of Pt SA/rGO toward HzOR is being investigated, with further efforts toward overall hydrazine splitting (OH₂S) for energy-efficient hydrogen production. In addition, Zn–hydrazine battery applications will be explored to demonstrate its potential for energy conversion and storage. This work presents a rapid laser-based strategy for constructing Pt single-atom catalysts and their potential application in hydrazine-based energy systems.

Keywords: Hydrazine Oxidation Reaction (HzOR); CO₂ Laser Process; Pt Single-Atom Catalysts; Hydrogen Production

Phase Selective K, Na and Li ion Storage behaviour of Copper Borates for Battery-type Hybrid Supercapacitors

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Abstract

Transition metal borates possess structurally diverse boron–oxygen frameworks that can strongly influence ion-storage behavior, yet their phase-dependent electrochemical properties remain underexplored. Herein, copper orthoborate (copper *o*-borate) and copper metaborate (copper *m*-borate) were synthesized through a rapid CO₂ laser-driven thermal-shock strategy enabling ultrafast phase-selective crystallization. Structural and spectroscopic analyses reveal distinct crystallographic and electronic characteristics between the two phases despite both predominantly containing Cu²⁺ species. Copper *m*-borate exhibits larger interplanar spacing, a higher fraction of bridging oxygen in polymeric borate units, a substantially lower work function than copper *o*-borate, and enhanced electronic excitation characteristics, suggesting more favorable ion diffusion and charge-transfer behavior. Electrochemical studies in KOH, NaOH and LiOH electrolytes reveal strong cation-dependent charge-storage behavior following the order KOH > NaOH > LiOH across various concentrations. Copper *m*-borate consistently outperforms copper *o*-borate, delivering a gravimetric capacitance (C_m) of 400.93 F g⁻¹ at 1 A g⁻¹, compared to 229.09 F g⁻¹ for copper *o*-borate. Dunn's method revealed that the battery-type intercalation-deintercalation was the predominant charge-storage mechanism, which is further supported by in situ Raman spectroscopy and time-of-flight secondary ion mass spectroscopy, highlighting the critical role of the borate framework in governing alkali-ion storage behavior.

Keywords: Copper borate, supercapacitors, intercalation-deintercalation, time-of-flight secondary ion mass spectroscopy, in situ Raman spectroscopy.

Investigation of Performance and Emission Characteristics for Green Nano-Flora-Fuel in the Direct Injection Diesel Engine

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Abstract

In the mutating automobile transportation technologies, biodiesel occupies a paramount share. Moreover, numerous renewable feedstocks are prominently contributing to biodiesel production. Metal oxide nanoparticles have enriched the flora fuels in recent days. Hence, indispensable demand raised for employing nanotechnology in the emission reduction of the compression ignition engine. Nanoparticles' utilization in the combustion fuel enhances the combusting nature. Succeeding the transesterification process, the methyl ester prepared from the kernel of tamarind seed (TSB) is used as biodiesel (20% blend ratio) to power the CI engine. The XRD, FTIR, UV, and PL spectra characterization of ZnO (ZnO NPs) nanoparticles have furnished the possibility of blending it with biodiesel. The ZnO (TSBN25 and TSBN50) nanoparticles (25 and 50 ppm) have shrunk the emission of toxic greenhouse gases (CO and HC-) below the emission level of metal oxide-less biodiesel. An increase in the volume of ZnO NPs has diminished the values of net heat release rate, peak cylinder pressure, and nitric oxide emission (NO_x). At the same time, the BTE of TSBN50 surged than the TSB. Analogously, exploiting the fuel additive, diethyl ether (TSBD) 10% with the biodiesel has subsided the NO_x levels, net heat release rate, in-cylinder pressure, and peak in-cylinder pressure. However, there was a hike in the mechanical efficiency of TSBD than the other combinations. The present investigation catalogues that the effects of diethyl ether and ZnO NPs are constructive in enhancing the performance and minimising diesel engine emissions.

Keywords: ZnONps, Nitric oxide emission, Tamarind seed, Diethyl ether.

Ce Incorporated Nis Electrocatalyst for Efficient Hydrogen Production Incorporation with Sugarcane Juice Oxidation Reaction

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Abstract

Energy-efficient electrolysis systems capable of simultaneous hydrogen production and biomass as feed is highly desirable for sustainable growth with no carbon emission and clean energy production. Herein, we report cerium-incorporated nickel sulfide (Ce-NiS) selfsupported electrocatalysts with single-step chemical bath deposition strategy for efficient hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and sugarcane juice oxidation reaction (SJOR). Ce-incorporation advances the electrocatalytic activity of NiS, promotes catalytically active oxy-hydroxy (NiOOH-) species, and reduces the interfacial resistance for effective charge-transfer kinetics. Consequently, Ce-NiS exhibits 100 mA/cm² at 1.33 V vs RHE for SJOR, lowering anodic potential by 300 mV as compared to OER and also effective energy reduction as compared to NiS. In-situ operando electrochemical impedance spectroscopy (EIS) and Raman spectroscopy reveal an indirect NiOOH-mediated oxidation pathway during SJOR. Leveraging its excellent bi-functional activity, a Ce-NiSbased electrolyzer is assembled for simultaneous hydrogen production and sugarcane juice electro-oxidation, requiring only 1.65 V to achieve 100 mA/cm², markedly lower than conventional alkaline water electrolysis (1.81 V). The sugarcane juice-assisted electrolyzer further achieves an ~8.7% reduction in electrical energy consumption for hydrogen production. Additionally, ¹H NMR and HPLC analysis confirm selective conversion of sugar-derived substrates into value-added formate with Faradaic efficiency of 85%. Present work highlights cerium modulated nickel sulfides as promising electrocatalysts for integrating effect of hydrogen generation with biomass valorization.

Keywords: Biomass-assisted electrolysis; sucrose electro-oxidation; hydrogen production; surface reconstruction.

Novel Zinc(II) Coordination Complex for Nonlinear Optics: Structural, Spectroscopic and SHG Insights

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Abstract

The study reports the synthesis of a new zinc complex, designated as ZnPDMCZ. The complex was studied using a combination of spectral and analytical tools, including UV–Visible spectroscopy, FTIR spectroscopy, ¹H NMR spectroscopy, ESI-MS spectrometry, TG-DTA analysis, and single-crystal X-ray diffraction (S-XRD). Crystallographic interpretation unveils that the ZnPDMCZ crystal belongs to the monoclinic system, non-centrosymmetric *Cc* space group, adopting a distorted octahedral coordination around Zn(II). Hirshfeld surface analysis evidences the non-covalent interactions, which govern the crystal packing and crystal stability. Density functional theory (DFT) computations estimate a dipole moment of 7.2226 D with first-order hyperpolarizability (30.4147×10^{-31} esu), suggesting the practicability of ZnPDMCZ for nonlinear optical (NLO) applications. The bulk NLO response was evaluated experimentally by SHG measurements, and the ZnPDMCZ crystal exhibited a measurable SHG efficiency of 0.15 relative to the standard KDP crystal.

Keywords: Zinc(II) complex, non-centrosymmetric crystal, Density functional theory, Dipole moment, Nonlinear optics.

Electrochemical Studies on B-MnO₂/Co₃O₄ Composite Material for Energy Conversion and Storage Technologies

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Abstract

The β -MnO₂/Co₃O₄ composite was successfully prepared through a facile single-step hydrothermal technique. Powder X-ray diffraction (XRD) analysis confirmed a highly crystalline composite nature with a tetragonal crystal system of the space group of I4₁/amd(No. 141). Scanning electron microscopy (SEM) studies revealed rod like β -MnO₂ nanostructures decorated by uniformly distributed Co₃O₄ nanoparticles. Electrochemical studies investigating the oxygen evolution reaction (OER) exhibit an overpotential of approximately 600 mV at 10 mA cm⁻² for this β -MnO₂/Co₃O₄ composite. Interestingly, prolonged electrochemical cycling resulted in enhanced oxygen evolution reaction (OER) activity and improved reaction kinetics, as evidenced by the variation in Tafel slope. These findings highlight the potential of β -MnO₂/Co₃O₄ composites for achieving improved oxygen evolution reaction (OER) stability and Kinetics. In addition, galvanostatic charge discharge (GCD) measurements were performed at different current densities to analyse their charge storage behaviour. The composite exhibited relatively 30 F/g specific capacitance values, indicating modest capacitive charge storage performance alongside its oxygen evolution reaction(OER) activity.

Keywords: Oxygen evolution reaction, Overpotential, galvanostatic charge discharge, specific capacitance.

Development of a Molecularly Imprinted ZnO–SiO₂ Photocatalytic Film for the Degradation of Bisphenol A

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Abstract

Molecular imprinting coupled with semiconductor photocatalysis offers a promising strategy for target-specific removal of organic contaminants from water. In this study, a bisphenol A (BPA)-imprinted ZnO–SiO₂ photocatalytic film was fabricated by a Sol–gel dip-coating method using zinc acetate dihydrate, TEOS, APTES, and BPA as the template. A non-imprinted (NI) film was prepared under identical conditions for comparison.

FTIR analysis supported formation of the functionalized siloxane network and template removal, while XRD confirmed hexagonal wurtzite ZnO dispersed within an amorphous silica-rich matrix, with a mean apparent crystallite size of 13.99 ± 0.74 nm. UV–Vis diffuse-reflectance analysis yielded an apparent direct optical band gap of approximately 3.11 eV.

At dark adsorption equilibrium, BPA adsorption was $23.63 \pm 2.06\%$ for the molecularly imprinted (MI) film and $10.00 \pm 0.66\%$ for the NI film, corresponding to an uptake-based imprinting factor of 2.36. After 150 min irradiation, apparent BPA removal was 97.66% for MI, 68.10% for NI, and 8.76% for light only. Pseudo-first-order rate constants were 0.024993, 0.008005, and $0.000640 \text{ min}^{-1}$, respectively, representing a 3.12-fold kinetic enhancement for MI over NI. These results demonstrate enhanced BPA rebinding and photocatalytic removal through molecular imprinting. However, the decrease in UV–vis absorbance represents apparent BPA removal or chromophore loss and does not independently confirm complete mineralization.

Keywords: Molecular imprinting; ZnO–SiO₂; Bisphenol A; Photocatalysis; Molecularly imprinted photocatalyst; Sol–gel; Water treatment

Magnetic-Ions (Nd^{3+} & Er^{3+}) Doping as a Pathway to Tuned Multiferroic and Magnetoelectric Properties in GdFeO_3

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Abstract

Multiferroic materials possessing simultaneous ferroelectric and magnetic orderings present immense potential for next-generation multifunctional devices, non-volatile memories, and energy storage applications. In this study, single-phase orthorhombic ($Pbnm$ space group) pristine GdFeO_3 (GDFO) and rare-earth-doped (Er^{3+} and Nd^{3+}) GDFO nanoparticles were successfully synthesized using a glycine-assisted auto-combustion method. Rietveld refinement and X-ray Photoelectron Spectroscopy (XPS) confirmed the precise ionic substitution at the Gd^{3+} sites without secondary phase impurities, alongside valence state verification and modulated oxygen vacancy concentrations. FESEM revealed distinct microstructural evolutions governed by dopant ionic radii: Er^{3+} substitution ($r_{\text{Er}^{3+}} < r_{\text{Gd}^{3+}}$) induced lattice distortion and unit cell volume contraction, yielding a uniform grain distribution (~ 51 nm for 50% Er), whereas Nd^{3+} doping ($r_{\text{Nd}^{3+}} > r_{\text{Gd}^{3+}}$) led to particle size enlargement. Electrical characterization demonstrated a significant reduction in leakage current density—by up to two orders of magnitude (10^{-7} to 10^{-9} A/cm² at 50 kV/cm for Nd-doping and one order for Er-doping) driven by reduced oxygen defect states while preserving ohmic conduction. Both dopants markedly improved dielectric permittivity (reaching ~ 920 for Er-doped compositions) via low-frequency space-charge polarization, alongside enhanced room-temperature ferroelectric polarization ($P_{\text{max}} = 0.123 \mu\text{C}/\text{cm}^2$ for 20% Nd). Magnetic measurements confirmed canted antiferromagnetism with augmented magnetization. Crucially, robust room-temperature DC magnetoelectric (ME) coupling was established, yielding maximum ME coefficients of 16.69 mV/cm · Oe for 50% Er and 14.44 mV/cm · Oe for 20% Nd accompanied by a 25% low-frequency magnetodielectric response (MDR). These findings demonstrate that tailoring GDFO via chemical pressure (doping) engineering unlocks strong room-temperature multiferroics suitable for multifunctional applications.

Weak Forces, Strong Architectures: Programming π -Space through Halogen Bonding

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Abstract

Halogen bonding represents a powerful noncovalent interaction for directing molecular recognition, crystal packing, and supramolecular assembly. However, how halogen bonding can be systematically exploited to control the organization and electronic properties of electron-deficient arylene imide and diimide π -systems remains largely unexplored. In this work, we investigate the halogen-bonding behavior of nine di-, tetra-, and octabrominated arylene imide/diimide derivatives based on phthalimide, pyromellitic diimide, naphthalenediimide, and perylenediimide scaffolds. By varying the π -scaffold size, axial substituents, bromination pattern, and imide heteroatom, we establish how molecular structure governs intermolecular interactions and supramolecular organization. Single-crystal X-ray diffraction reveals a diverse range of $\text{Br}\cdots\text{O}$, $\text{Br}\cdots\text{Br}$, and $\text{Br}\cdots\pi$ interactions, leading to the formation of cyclic halogen-bonded motifs and extended one- and two-dimensional architectures, including corrugated sheet-like assemblies. $\text{Br}\cdots\text{O}$ contacts are found to dominate the crystal structures, whereas $\text{Br}\cdots\pi$ interactions become prominent in systems containing axial mesityl groups and conformationally distorted arylene diimide cores. These structural variations are accompanied by significant modulation of the electronic properties, with reduction potentials ranging from -1.09 to -0.17 V versus SCE and LUMO energies reaching approximately -4.2 eV. Hirshfeld surface, AIM, and NBO analyses further establish the structural and electronic origins of these interactions, revealing predominantly closed-shell halogen bonds and donor–acceptor interactions involving lone-pair orbitals and $\sigma^*(\text{Br}-\text{C})$ orbitals. The greater stabilization associated with $\text{Br}\cdots\text{O}$ contacts provides further insight into the preferential formation of these interactions. Overall, our results demonstrate that halogen bonding can serve as an effective molecular-level tool for controlling crystal packing, supramolecular assembly, and electronic properties in electron-deficient π -systems. This study provides a foundation for designing higher-order halogen-bonded architectures with potential applications in supramolecular materials, organic electronics, and nonlinear optical materials.

CNT modified Self-Sustainable Flexible Energy Device

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Abstract

Flexible and sustainable energy-storage technologies require electrode architectures that can simultaneously support efficient ion transport, mechanical adaptability, and reliable operation under demanding environmental conditions. In this work, we develop a screen-printable CNTbased micro-supercapacitor by regulating the intertubular structure of CNT inks through Li⁺ incorporation. The modified CNT network provides enlarged ion-accessible pathways, while a LiTFSI water-in-salt electrolyte offers a broad electrochemical operating window and facilitates efficient charge storage. The resulting interdigitated microsupercapacitor delivers an areal capacitance of 42 mF cm⁻² with approximately 95% capacitance retention over 20,000 charge– discharge cycles. Importantly, the device retains stable electrochemical characteristics at temperatures and exhibits humidity-responsive energy-generation capability. The printed devices also demonstrate good reproducibility and mechanical flexibility, highlighting the robustness of the proposed electrode–electrolyte architecture. These results demonstrate a scalable strategy for developing flexible microsupercapacitors capable of reliable energy storage and operation under variable environmental conditions.

Keywords: Carbon, Flexible, Energy, Micro-supercapacitor.

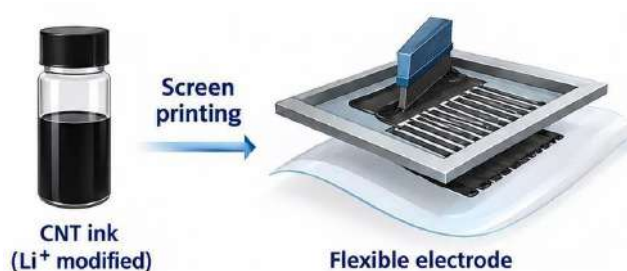


Figure: Fabrication of CNT based flexible electrode using screen printing.

Electrochemical Investigation of Molybdenum Trioxide with Enhanced Charge Storage Capability for Supercapacitors

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Abstract

The growing concerns over fossil fuel depletion and environmental degradation have stimulated extensive research into sustainable and efficient energy storage technologies. Supercapacitors have emerged as promising energy storage devices owing to their high power density, long-term cycling durability, and superior rate capability. In particular, the selection and design of suitable electrode materials are of paramount importance in enhancing their electrochemical charge storage performance. In this study, molybdenum trioxide based positive electrode has been designed and its electrochemical performances including cyclic voltammetry and galvanostatic charge-discharge are evaluated using three-electrode configuration through aqueous electrolyte. Interestingly, the molybdenum trioxide electrode exhibits remarkable electrochemical performance, characterized by a prolonged discharge time, which can be attributed to its enhanced charge storage capability and highly reversible redox activity. It can be due to the layered structure, high surface-to-volume ratio, multiple electroactive sites, and superior faradaic redox mechanisms of molybdenum trioxide.

Keywords: Supercapacitors, Molybdenum trioxide, Charge-Discharge, Redox reaction.

Design and Development of a Portable Solar-Powered Mobile Charging System

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Abstract

The increasing use of mobile devices has created a need for portable and reliable charging solutions. In this research work, a solar powered mobile phone charger was designed and constructed using a photovoltaic panel, rechargeable battery and voltage regulating circuit. The system converts solar energy into electrical energy and stores it in a battery for later use. A buck converter is used to regulate the voltage and provide a stable 5V output suitable for charging mobile phones through a USB port. The developed prototype demonstrates that solar energy can be used as an eco-friendly and cost-effective alternative for charging electronic devices, especially in areas where electricity supply is limited or unavailable.

Keywords: Solar charger, Photovoltaic panel, Buck converter, and Mobile phone charging.

Use of Sugarcane as a Bioenergy Crop: Sustainable Energy Solutions

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Abstract

The increasing demand for energy, combined with the environmental impacts of fossil fuels, has created an urgent need for renewable and sustainable energy sources. Biomass is an important renewable resource, and sugarcane is one of the most promising crops for sustainable bio-energy production. Sugarcane can produce energy not only from its sugar content but also from its agricultural and industrial residues, including bagasse, molasses, straw, and vinasse. These materials can be converted into bioethanol, electricity, heat, biogas, biohydrogen, and other value-added products. Sugarcane bagasse is particularly important because it is a lignocelluloses residue that can be used for cogeneration, second-generation ethanol production, and biogas generation. In India, sugarcane bagasse is available in large quantities, creating significant opportunities for integrated biorefineries and rural sustainable development. However, challenges such as high water requirements, seasonal availability, biomass transportation, pretreatment costs, and technological limitations must be addressed. This paper examines the role of sugarcane as a bioenergy crop, major conversion technologies, environmental and economic benefits, challenges, and future opportunities. The study concludes that integrated sugarcane biorefineries can contribute significantly to sustainable energy systems, circular economy development, waste reduction, and reduced dependence on fossil fuels.

Keywords: Sugarcane, Bioenergy, Bioethanol, Bagasse, Biomass, Biogas, Sustainable Energy, Biorefinery, Renewable Energy.

Processing of AA2014 Reinforced with Tungsten Disulfide and Molybdenum Disulfide Nano Particles through Stir Casting

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Abstract

The development of hybrid metal matrix composites with suitable reinforcement is a challenging one since the industries expect superior performance for their products with significant improvements in their properties. As a result, composite materials are in demand. In this study, an aerospace aluminium alloy (AA2014)-based hybrid composite material was processed through a stir casting process with the nano-sized reinforcement of tungsten disulfide (W_2S) and molybdenum disulfide (MoS_2). After the solidification, it was noted that the cast samples were successfully made with no defects. Further, the sample was subjected to morphological and elemental analysis studies through scanning electron microscopy (SEM) and energy dispersive x-ray spectroscopy (EDS). The results show that the reinforcements were well dispersed into the aluminium matrix. Al_2Cu precipitates were found in the composite. W_2S addition improves its self-lubricating surface, vacuum stability and load-carrying capacity. MoS_2 particles function as solid lubricants and introduce some changes in their structural properties. The addition of both reinforcement and nucleation during solidification and recrystallisation resulted in substantial grain refinement. Some agglomeration was also found because of MoS_2 particles and it formed weak zones that may induce microcracking when the applied load increases. The microstructural changes may be qualified rely on the percentage of contribution of reinforcement and the processing route.

Keywords: AA2014, hybrid composite, SEM, Tungsten Disulfide

Molecular Structure and Stability of New Carbon and Boron Allotropes C_n Where $N = 24, 32, 40$ And 48 – A Theoretical Study

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Abstract

Carbon is termed as “THE KING OF ELEMENTS”, as it is capable of forming many allotropes due to the valency of carbon and it forms chains very easily. Carbon forms different types of allotropes like amorphous carbon, single-walled carbon nanotube, bucky tube, nanobuds, nanoribbons, C_{60} (buck minister fullerene (or) bucky ball), C_{540} , C_{70} , graphite, lonsdaleite, diamond, fullerenes, nanotubes and so on which arises out from its various bonding models which includes sp , sp^2 and sp^3 . Due to the variation in the structures, the allotropes of carbon have distinct behavior on the same properties like thermal stability, conductivity, absorption, crystallinity, strength, flexibility, optoelectronic properties and so on.¹ Computational chemistry tools like Density Functional Theory (DFT) have already been used successfully to identify and predict the stability of novel carbon allotropes $C_{24}(oh)$, fcc- C_{10} , fcc- C_{12} , bcc- C_{20} , and fcc- C_{32} . Here we have used DFT (BP86/Def2-TZVP) method to predict the possibility of new carbon allotropes C_{24} , C_{32} , C_{40} and C_{48} .

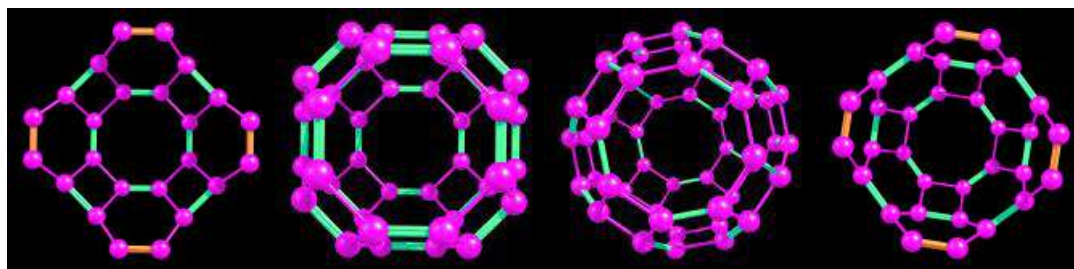


Figure: DFT (BP86/TZVP) optimized geometries of C_{24} , C_{40} , C_{48} , and C_{32}

DFT is used to determine the properties of a compound that includes molecular geometries, exchanges of energies, hydrogen bonding and other intrinsic properties. Our initial results predict the possible stability of the allotrope C_{32} . DFT computed bond parameters are in agreement with already known similar compounds. The important results obtained will be presented.

OP-EN-27

Influence of Transition Metal (Fe) doped Zinc Oxide (ZnO) Nanoparticles

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Abstract

Nanotechnology is characterised as the development and application of materials on the smallest scale possible. Diagnostics, drug distribution, sunscreens, antimicrobial, disinfectants, an environmentally sustainable engineering process that eliminates waste products (zero waste), as a catalyst for greater productivity in current industrialized processes by minimising or eliminating the use of hazardous materials, to minimize pollution and an greener energy production. The selected material ZnO (metal oxide) is a chemically and thermally stable n-type II–VI compound semiconductor materials with wide band gap energy of 3.37 eV and a high exciton binding energy about is 60 meV, which have been refer to plenty of applications. The Co-precipitation method (CPM) was used to make pure and Fe doped Zinc Oxide (ZnO) nanoparticles (Nps) in this study. X-ray diffractometer (XRD), UV–vis absorption spectroscopy and Fourier transform infrared spectroscopy (FTIR) were used to describe the sample's structural, optical, and electrical properties. The hexagonal wurtzite structure of ZnO was verified by the X-ray diffraction pattern. The Debye-Scherrer formula was used to measure the average crystallite size. The pure and Fe doped ZnO sample absorbs the radiations in the UV ranges up to 327.27, 324.74 and 323.5 nm and almost all the visible spectrum radiations are transmitted by the synthesized Nps. FTIR analysis was used to identify the functional frequencies of pure and Fe doped ZnO Np. The electrical conductivity of ZnONps decreases with Fe doping concentration due to increase in deep donor concentration. The Surface morphology of the pure and Fe doped zinc oxide nanoparticles studied by Scanning Electron Microscopy (SEM).

Keywords: ZnO Np's Co-precipitation, X-ray diffractometer, Optical properties, Electric conductivity

Phytosynthesis of Copper Nanoparticles using *Psidium guajava* and Testing their effects on *Vigna Unguiculata* Seed Germination

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Abstract

This research looked at how copper oxide (CuO) nanoparticles, produced through green synthesis methods, influence seed germination and early growth in *Vigna unguiculata*. The guava fruit extract served as the reducing and capping agent for the CuO nanoparticles. A combination of techniques, including UV-Vis spectroscopy, DLS, XRD, FTIR, SEM, and EDX, was used to confirm that the nanoparticles had formed correctly and retained their structural integrity. Seeds were treated (nanoprimered) with different concentrations of each nanoparticle type, and researchers then tracked several growth indicators: germination rate, seedling vigour, shoot and root development, leaf size, biomass, and chlorophyll levels. The results revealed clear dose-dependent trends. CuO nanoparticles worked best at a low concentration of 0.2 ppm, where they noticeably boosted germination, vigour, overall growth, and biomass production. Statistical testing confirmed these differences between treatments were meaningful. Overall, the study points to green-synthesized nanoparticles as a promising, eco-friendly approach to seed priming, while also making clear that getting the dosage right matters—too much can tip the balance from beneficial to harmful.

SnS₂@MWCNT Hybrid Electrodes with Enhanced Charge Storage for High-Performance Asymmetric Supercapacitors

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Abstract

The current study investigates the extraordinary electrochemical properties of tin sulphide integrated with multi-walled carbon nanotubes (SnS₂@MWCNTs) synthesised using a simple and easily repeatable hydrothermal process. The tight interaction of SnS₂ particles with carbon nanotubes creates a seamless conductive framework, significantly improving charge mobility and electrical conductivity within the composite. XRD, SEM, and XPS analysis of SnS₂@MWCNTs' architecture and surface validates their successful manufacture. The synthesised SnS₂@MWCNT composite outperformed pure SnS₂, with a peak capacitance of 1666 Fg⁻¹ at a current density of 1 Ag. A device with an aqueous asymmetric capacitor (ASC) was created employing the SnS₂@MWCNT composite for the cathode and activated carbon (AC) electrodes for the anode, resulting in an energy density of 56 Whkg⁻¹ and a power density of 725 Wkg⁻¹. In addition, when two SnS₂@MWCNTs cells were coupled in series, the collected energy was enough to power two yellow LEDs in parallel. This composite material is projected to significantly enhance future electrical energy storage systems and other electronic devices.

Keywords: SnS₂, MW-Carbon nanotubes, Hydrothermal synthesis, Hybrid supercapacitor, Electrochemical energy storage

pH-Functionalized Metal-Free Carbon Dots as White Phosphors for Cool White LED Applications

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Abstract

Carbon dots (CDs) have emerged as versatile zero-dimensional carbonaceous nanomaterials owing to their distinctive photoluminescence, facile preparation, and tunable physicochemical characteristics. Their low toxicity and cost-effective synthesis further enhance their suitability for emerging optoelectronic applications. In particular, the development of a single component carbon dot phosphor capable of generating white light is highly desirable for next generation solid state lighting, as it can simplify the conventional phosphor architecture used in light-emitting diodes (LEDs). Although rare-earth based phosphors are widely employed for white-light generation, their complex synthesis and high material cost restrict their practical applicability. In response to this, we explored reproducible, single-step hydrothermal strategy for preparing white-light-emitting carbon dots using L-leucine and L-tryptophan under pH-assisted reaction conditions. The resulting CDs displayed a photoluminescence profile with a maximum emission centered at 450 nm. To construct a stable colour-conversion layer, the CDs were incorporated into a polyvinyl alcohol (PVA) matrix, which effectively limits nanoparticle aggregation and the associated self-quenching of photoluminescence. The resulting CD/PVA phosphor film was subsequently integrated with a 365 nm ultraviolet LED to demonstrate white-light generation. Notably, the phosphor film retained its emission characteristics for up to 300 days under room-temperature storage with a decay lifetime of 18.6 ns. The fabricated device exhibited a high colour rendering index (CRI) of 86%, with CIE chromaticity coordinates of (0.302, 0.318) and a correlated colour temperature (CCT) of 7236 K, corresponding to cool white emission located close to the Planckian locus. These findings demonstrate the potential of synthesized CDs as stable, efficient and metal-free phosphors, offering a promising route towards economical cool white LED technology.

Keywords: White phosphor, Light emitting diodes, Carbon dots, Amino acids, Hydrothermal, Photoluminescence

Tribological Performance of Chemically Modified Jatropha and Pongamia Oil Blends as Alternatives to Mineral Lubricant

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Abstract

This paper investigates chemically modified non-edible Jatropha and Pongamia oils blended with SAE 20W40 mineral oil as potential sustainable lubricants. Crude oils were chemically modified through twostep acid–base transesterification followed by reaction with trimethylolpropane (TMP). The modified oils were blended at 3%, 9% and 12% by volume and evaluated against neat mineral oil using a pin-on-disc tribometer. Tests covered loads of 40–200 N, sliding speeds of 300–1500 rpm, 150°C temperature, an 80 mm wear track and 30,000 m sliding distance. Coefficient of friction, and specific wear rate were measured, while optical microscopy and SEM were used for surface characterization. The 3% and 9% Jatropha and Pongamia blends generally reduced friction, and wear compared with mineral oil, whereas 12% blends showed deterioration. Jatropha blends generally provided better wear resistance than Pongamia blends. The findings indicate that controlled low-concentration chemically modified nonedible oil blends can provide a promising route toward more sustainable lubrication.

Keywords: Jatropha oil; Pongamia oil; biolubricant; mineral oil; friction; wear; pin-on-disc.

Mechanistic Investigations on the Redistribution Reactions of Tin Compounds – A DFT Study

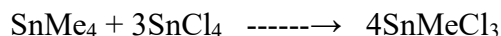
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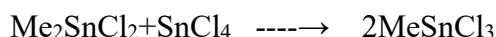
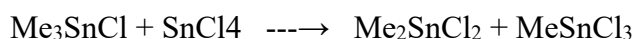
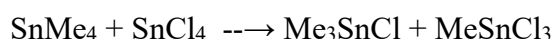
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Abstract

Tin compounds are possessing potential applications in various fields like energy storage, solar cells, gas sensors, thermoelectric devices, antimicrobial and anticancer agents etc. Organotin compounds are those containing at least one Sn-C bond. Tin with the electronic structure of [Kr] $5s^25p^2$, possess the oxidation states +2 and +4, and exhibit a variety of chemistry. Tin complexes are known for the coordination numbers ranging from 2 to 12 showing diverse structural features and reaction mechanisms, although experimental tin chemistry is well explored, many areas of tin chemistry merits theoretical investigations. Tin compounds have many applications, such as catalysis, agrochemicals and as potential antitumor agents. Following our previous work, we are investigating the redistribution reaction of



which proposed to occur in three steps viz.,



DFT calculations have been performed to study the structure, bonding, reaction mechanisms and thermodynamic properties of the above-mentioned reactions.

Keywords: Tin, DFT, Redistribution reaction, Bonding.

Element-Specific Magnetic Interactions in Mn/Cr Double-Doped CdTe Thin Films for Spintronic Applications

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Abstract

Transition-metal (TM) co-doping provides an effective approach for engineering the structural, electronic, optical, and magnetic characteristics of II-VI semiconductor materials, offering new opportunities for multifunctional and spintronic applications. The structural, surface morphological, optical, and magnetic characteristics were examined using X-ray Diffraction (XRD), High-resolution Scanning Electron Microscopy (HR-SEM), Atomic Force Microscopy (AFM), Fourier-Transform Infrared Spectroscopy (FTIR), Photoluminescence (PL), Vibrating Sample Magnetometry (VSM), X-ray Absorption Spectroscopy (XAS), and X-ray Magnetic Circular Dichroism (XMCD). The XRD analysis confirms the cubic zinc blende structure of CdTe without any secondary peaks, which confirms the successful doping of Mn and Cr into the Cd lattice in CdTe. HR-SEM and elemental mapping further demonstrate a uniform surface morphology and homogeneous distribution of the constituent elements, confirming the good structural quality and compositional uniformity of the deposited films. Element-selective XAS and XMCD measurements provide direct evidence for the evolution of magnetic ordering upon Cr incorporation, demonstrating a transition from paramagnetic behavior in Mn-doped CdTe toward pronounced ferromagnetism in the Mn-Cr co-doped system. This magnetic enhancement is associated with the interaction between localized $\text{Mn}^{2+}/\text{Cr}^{2+}$ 3d states and the charge carriers of the CdTe host, mediated by double-exchange mechanisms and strong *sp-d* exchange coupling. The incorporation of Cr modifies the electronic structure and strengthens the magnetic exchange interactions, thereby promoting stable ferromagnetic ordering at room temperature. These findings demonstrate that Mn-Cr codoped CdTe thin films possess enhanced magnetic functionality and represent promising materials for the development of next-generation spintronic and magneto-electronic devices.

Keywords: Dopants, CdTe, XAS, XMCD, Spintronics

Orbital magnetic moment enhancement in NiFe_2O_4 thin films probed by X-ray magnetic circular dichroism

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Abstract

In this work, we report the effects of substrate temperatures on the structural, morphological, electronic, and magnetic characteristics of nickel ferrite (NiFe_2O_4) thin films produced by spray pyrolysis. An inverse spinel structure with increased crystallinity was verified by X-ray diffraction (XRD). High-resolution scanning electron microscopy (HR-SEM) and Energydispersive spectroscopy (EDS) were used to analyse morphology and elemental composition. Vibrating Sample Magnetometry (VSM), X-ray Absorption Spectroscopy (XAS), and X-ray Magnetic Circular Dichroism (XMCD) were used to investigate the magnetic and electronic characteristics at room temperature. VSM revealed ferrimagnetism and magnetic anisotropy effect in NiFe_2O_4 . XAS and XMCD show Ni^{2+} ions in octahedral sites, with Ni^{2+} spins more affected by structural defects, leading to spin canting through spin-orbit coupling, and Fe^{3+} ions in tetrahedral and octahedral sites. We obtained orbital magnetic moments of $0.115 \mu_B/\text{ion}$ for Ni and $0.243 \mu_B/\text{ion}$ for Fe, driven by structural distortions and Fe 3d–O 2p hybridization. The obtained results are particularly interesting for spintronic applications.

Keywords: NiFe_2O_4 thin films, X-ray Absorption Spectroscopy, X-ray Magnetic Circular Dichroism, Orbital magnetic moment, Spintronic applications

Nanoengineered Electrodes for Microbial Fuel Cells: Toward Sustainable Energy Systems

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Abstract

Microbial fuel cells (MFCs) are emerging bioelectrochemical platforms for simultaneously producing renewable energy and treating wastewater. Despite significant research endeavors, the widespread commercialization of MFC technologies has been hampered by the issues of low power outputs, slow oxygen reduction rate and sub-par system longevity. The tremendous breakthroughs achieved in the areas of nanomaterial science over the past decades have dramatically elevated the performance of MFCs via the facilitation of efficient electron transfer, microbial-cell adherence, cathodic oxygen reduction process and membrane stability. Nanostructured carbon materials including carbon nanotube, graphene offer high electrical conductivity, maximized electrochemically active surface area; can be utilized to design highperformance anodes, whereas transition metal-based catalyst-including FeNC, MnO and CoO nanoparticles can be employed as inexpensive substitutes for platinum cathodes. Nanomembranes made from silica, graphene oxide and TiO₂ can simultaneously boost the transportation of protons, shield microbes from invasion and fungi, and boost the lifespan of MFC systems. Nanomaterial-based MFCs have not only been studied as green power supplies, but also as effective means to remediate wastewaters, monitor the bioelectric signals, concurrently produce biohydrogen, as well as facilitate off-grid decentralized energy systems. Nonetheless, some challenges such as high cost, nanoparticle toxicity, and lack of standard testing procedures still need to be addressed. Challenges and future directions include the synthesis of environmentally benign nanomaterials, the fabrication of three-dimensional nanostructured electrodes, the combining of nanomaterials with IoT and intelligent algorithms to create smart sensing, and the design of circular bioeconomy-related MFCs.

Keywords: Microbial Fuel Cells (MFCs), Nanomaterials, Electrode Engineering, Carbon Nanotubes, Graphene, Bio electrochemical Systems, Sustainable Energy, Wastewater Treatment

Electrochemical Behavior and Nano Film Characteristics of Xylitol chelated Green Electroless Copper Deposition Stabilized by Mercapto pyridine

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Abstract

Technological advancements and discoveries have made advanced electroless plating into an indispensable asset for numerous industries, serving several modern applications. In this study, xylitol, a naturally occurring polyol, is explored as a green chelator for the preparation of nano copper film coatings through the electroless deposition process. The proposed research work aims at preparation and optimization of a sustainable plating bath by replacing conventional hazardous chelator EDTA with xylitol, which is biodegradable, nontoxic, and reduces environmental footprint. Xylitol manages the oxidation-reduction reaction rate, stabilizes metal ions leading to smoother, more uniform nucleation and crystal growth on the substrate surface. This work has employed DMAB as the reducing agent and mercapto pyridine as the stabilizer in the electroless bath. The addition of mercapto pyridine has resulted in the bath stabilization and grain refinement of the nano copper deposits. This study highlights the electrochemical and physical characteristics of the electroless plating bath and the resultant nano copper deposits. The nano copper deposits were characterized using XRD and SEM techniques. Cyclic voltammetric and impedance studies were carried out to assess the electrochemical characteristics of the electroless deposition baths.

Keywords: Xylitol, sustainable, nano copper, DMAB, mercapto pyridine.

Boosting Selective CO₂ Electroreduction via MXene-BiCuS Interfacial Engineering

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Abstract

The electrocatalytical reduction of carbon dioxide to value-added products is a promising strategy for achieving a sustainable carbon loop. Herein, a series of Bi-Cu bimetallic sulfide loaded on Ti₃C₂MXene (BCS@MXC) composites catalysts were synthesized via a facile self-impregnation deposition approach. The as-synthesized catalysts were well characterized via various analytical and spectroscopic techniques and followed for eCO₂RR. The 2-BCS@MXC catalyst presented excellent electrochemical activity with a high current density of -34.91 mA/cm² and a lower potential of -0.6 V vs. RHE in 0.1 M KHCO₃ electrolyte for eCO₂RR. The Electrochemical measurements were carried out in 3-electrode cell with the catalyst loading of 0.64 mg/cm². The 2-BCS@MXC catalyst exhibited the excellent selectivity for HCOOH with a Faradaic efficiency of 87.25% at an optimal potential -0.6 V vs. RHE. The 2-BCS@MXC showed a low charge transfer resistance (R_{ct}) of 16.37 Ω at an applied potential of -0.59 V vs. RHE and a higher C_{dl} value of 5.27 mF cm⁻², revealing the better reaction kinetics and higher electrochemically active surface area. The 2BCS@MXC could operate upto 37 h without loss in current density, showing better stability of the catalyst. Sulfur incorporation into the BCS@MXC lattice played a pivotal role in promoting H* formation, stabilizing the HCOO* intermediate for the formation of HCOOH, and enhancing catalytic activity. This study highlights the potential of structural engineering in MXene-based catalysts and highlights BCS@MXC as a promising material for efficient CO₂RR to value-added products; also it can be used in other energy and environmental applications.

Keywords: Ti₃C₂MXene, bimetallic effect, BiCuS, eCO₂RR

Influence of ZnO Incorporation on the Structural, Optical, and Electrical Properties of TiO₂/SnO₂ Thin Films

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Abstract

In this study, the effect of incorporation of ZnO on the structural, optical, surface morphological and electrical properties of TiO₂/SnO₂ thin films has been investigated for possible optoelectronic applications. TiO₂/SnO₂ and TiO₂/SnO₂/ZnO mixed metal oxide thin films were deposited on glass substrates using the electron beam evaporation technique with an average thickness of 250 nm. The phase composition and crystallinity of the films were determined by XRD analysis. The inclusion of ZnO changes the diffraction properties of the TiO₂/SnO₂ suggesting changes in crystallinity and microstructural ordering. UV-Vis absorption measurements showed a clear modification of the absorption edge after ZnO incorporation. The optical bandgap was calculated using the Tauc relation and the obtained values ranged from 4.10 eV for TiO₂/SnO₂ to 4.18 eV for TiO₂/SnO₂/ZnO, suggesting the ability of ZnO inclusion to modulate the electronic structure of the composite film. I-V measurements confirmed the semiconducting behavior of both films, and the Hall measurements gave quantitative information on the carrier concentration, mobility, resistivity and conductivity. The TiO₂/SnO₂ film showed a carrier concentration of $1.58 \times 10^{18} \text{ cm}^{-3}$, mobility of $33 \text{ cm}^2/\text{V}\cdot\text{s}$, resistivity of $11.59 \times 10^{-2} \Omega\cdot\text{cm}$, and conductivity of $8.62 \Omega^{-1}\cdot\text{cm}^{-1}$. With ZnO incorporation, these values changed to $1.65 \times 10^{18} \text{ cm}^{-3}$, $34 \text{ cm}^2/\text{V}\cdot\text{s}$, $10.87 \times 10^{-2} \Omega\cdot\text{cm}$ and $9.19 \Omega^{-1}\cdot\text{cm}^{-1}$, respectively. These changes indicate that ZnO incorporation enhances the charge-transport characteristics of the TiO₂/SnO₂ thin film. AFM analysis was used to investigate the surface topography, grain distribution, and root-mean-square roughness. A significant increment of the roughness parameters ($R_a = 6.80 \text{ nm}$, $R_q = 11.8 \text{ nm}$) has been obtained upon ZnO incorporation in TiO₂/SnO₂ thin film. The obtained TiO₂/SnO₂/ZnO heterostructure with adjustable bandgap, tailored surface morphology and tunable charge-transport properties is promising for optoelectronic technologies, such as UV photodetectors, transparent electronic components, optical sensors and electron-transport layers in photovoltaic devices.

Keywords: Thin Film, XRD, UV-Vis, I-V Characteristics, Hall Measurements, AFM.

Interfacial engineering of CoFe₂O₄/MnWO₄ heterojunctions for the ultrasound assisted photocatalytic degradation of sulfamethazine

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Abstract

The widespread presence of antibiotics in aquatic environments poses escalating ecological and public health challenges due to their persistence and contribution to antimicrobial resistance. Sulfamethazine (SMZ), a sulfonamide antibiotic, exhibits high environmental stability because of its rigid aromatic ring structure, strong hydrogen bonding, and tautomeric activity, rendering it resistant to conventional remediation methods. Herein, a cobalt ferrite/manganese tungstate (CFO/MWO) heterojunction with an S-scheme configuration is fabricated *via* a solid-state approach to attain high-performance sonophotocatalysis. Under optimal conditions, the CFO/MWO catalyst attains about 93% SMZ degradation in 60 min, featuring a rate constant of 0.00195 min⁻¹. The present process outperforms the individual sonocatalytic and photocatalytic systems by 11 and 7 times, respectively, achieving a synergistic factor of 1.75. X-ray Absorption Spectroscopy (XAS) analysis confirms the existence of redox reactions of Co²⁺/Co³⁺, Fe²⁺/Fe³⁺, and Mn²⁺/Mn⁴⁺ ions, indicating active participation in the degradation mechanism. Density Functional Theory (DFT) calculations prove that there is electron transfer and reactive oxygen species formation between the interfaces of CFO/MWO heterojunctions and catalytically active sites. Furthermore, the zebrafish embryo assays show low toxicity of the degraded sample. These findings demonstrate that CFO/MWO heterostructure-based nanomaterials serve as promising candidates for sustainable water treatment applications.

Keywords: Sulfamethazine, Cobalt ferrite, Zebrafish, X-ray absorption spectroscopy

Contact-Barrier Modulation of Self-Powered and Bias-Assisted Photodetection in pSi/n-SnSSe Heterojunctions

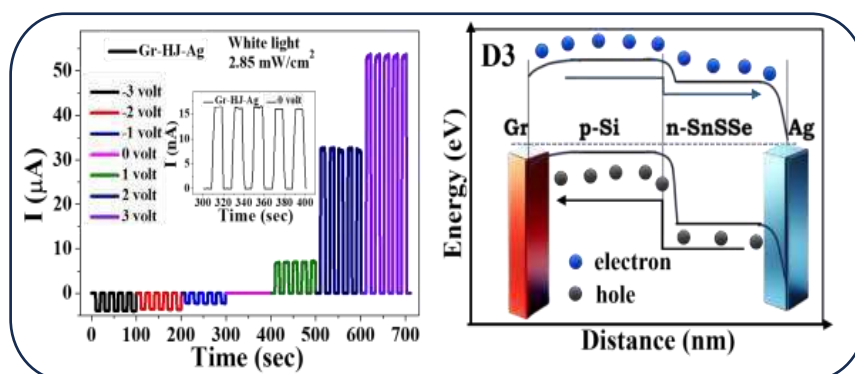
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Abstract

Broadband photodetectors that combine zero-bias operation with high responsivity under applied bias require simultaneous control of heterojunction band bending and carrier-selective contacts. Here, the influence of electrode symmetry and work-function contrast on spray-coated p-Si/n-SnSSe heterojunction photodetectors is investigated using Ag (4.28 eV) and graphene (4.70 eV) contacts. Four architectures were compared: Ag/HJ/Ag (D1), Gr/HJ/Gr (D2), Gr/HJ/Ag (D3), and Ag/HJ/Gr (D4). The complementary absorption of p-Si and few-layer n-SnSSe produced broadband photodetection from 505 to 940 nm, while the electrode configuration independently regulated the contact barriers and the net internal potential gradient. D3 exhibited self-powered operation, generating a photocurrent of 16.6 nA at zero bias under white-light illumination. This behaviour originates from the Ag/graphene workfunction contrast, which reinforces



directional separation and collection of photogenerated carriers without an external field. Conversely, D4 delivered the strongest bias-assisted performance at 635 nm under 130 $\mu\text{W}/\text{cm}^2$ illumination and +3 V, with a responsivity of 1.01 A/W, external quantum efficiency of 197.29%, and specific detectivity of 3.75×10^{11} Jones. Under forward bias, the applied field promotes hole transport across the Ag/p-Si barrier, while the graphene/n-SnSSe contact supports electron extraction; trap-mediated carrier-lifetime extension additionally produces photoconductive gain. The asymmetric devices also showed reproducible photoswitching, with rise/fall times of 0.43/0.28 s for D3 and 0.59/0.58 s for D4. These results distinguish two contact-controlled operating regimes: photovoltaic carrier separation in D3 at zero bias and field-assisted photoconductive amplification in D4 at positive bias. The solution-processed, lithography-free architecture therefore provides a scalable route to energy-efficient broadband photodetectors whose operating mode can be selected through electrode ordering rather than modification of the active heterojunction.

Keywords: SnSSe, p-Si heterojunction, photodetector, asymmetric electrodes, self-powered operation, broadband photoresponse

Experimental, electrochemical, and morphological investigations of Limonia Acidissima Rind extract as a green corrosion inhibitor for mild steel in 3.5% NaCl medium

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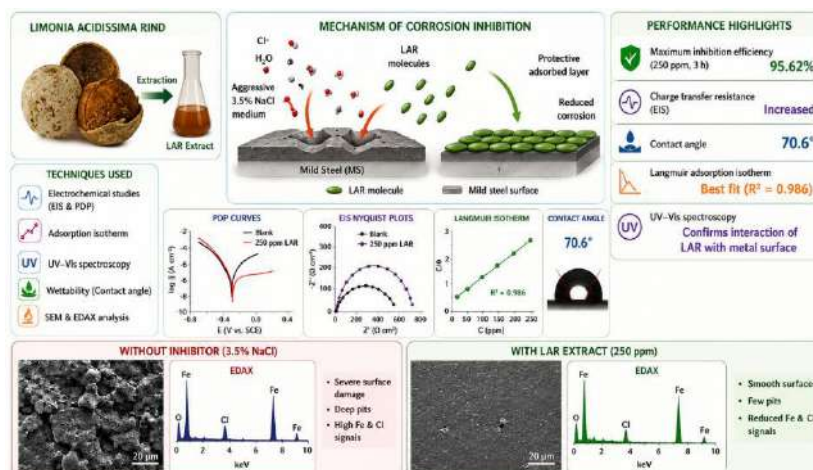
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Abstract

The Corrosion protection potential and surface adsorption behaviour traits of Limonia Acidissima Rind (LAR) extract for mild steel in 3.5% NaCl medium have been inquired utilizing SEM, EIS, PDP, Adsorption isotherm, UV–vis spectroscopy, and wettability through contact angle analysis. Notably, incorporating LAR, especially at a high dosage of 250 ppm, significantly mitigated oxidation, attaining a remarkable protective proficiency of 95.62% in 3 h. Adsorption analyses revealed that Langmuir isotherm showed a superior fit ($R^2 = 0.986$), indicating LAR adsorption on a mild steel surface at 298 K. Electrochemical impedance spectroscopy further validated the inhibitor's ability to form a protective barrier against corrosion. The contact angle of 70.6° of MS with inhibitor demonstrates that the rind extract increases the hydrophobicity of mild steel and enhances its resistance to corrosion. UV–Vis spectroscopy shows that LAR is an effective corrosion inhibitor, forming a protective interaction with the metal surface. SEM imagery revealed diminished surface degradation and fewer corrosive pits, affirming LAR's efficacy in preserving the integrity of mild steel under 3.5% NaCl.

Keywords: Corrosion, Limoniaacidissima rind, Inhibitor, Extract, Mild steel, Polarization



Development of a Magnetic Spring Generator for Sustainable Ocean Wave Power Generation: Design, Simulation, and Performance Analysis

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Abstract

This paper presents the design, mathematical modeling and simulation-based performance evaluation of a small-scale ocean wave energy harvesting system based on a magnetic spring generator. The proposed system consists of a floating buoy and a permanent magnet attached to the buoy. The vertical oscillatory motion of the buoy is converted into electrical energy by relative motion between the magnet and a stationary coil. The mechanical dynamics of the buoy-magnet assembly are modeled by a mass-spring-damper formulation, and the resulting motion is used to estimate the induced electromotive force (EMF) in the coil. Simulation results obtained by means of OpenModelica simulations under sinusoidal wave-like forcing of the buoy show stable oscillatory motion with a natural frequency of about 2.5 Hz. The generated AC voltage is in the range of 0.5 V to 3 V, and the smoothed DC output voltage after rectification and filtering is in the range of 0.5 V to 2 V. The estimated conversion efficiency of the proposed prototype-scale system is in the range of 60% to 70%. The proposed system offers a low-cost and low-maintenance alternative to conventional turbine- and hydraulic-based wave energy conversion systems. It can be easily scaled up by means of multi-buoy arrays to provide higher aggregate power. Therefore, it is a promising option for decentralized power supply in coastal and island communities.

Key words: Ocean wave energy, magnetic spring generator, electromagnetic induction, mass-spring-damper model, OpenModelica, renewable energy, wave energy converter (WEC).

Colloidal Engineering-driven Surface Stabilization of PbS NPs using Hydrophilic Spacer-based Cationic Gemini Surfactants: Structure–Function Relationships

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Abstract

Biologically derived surface-stabilizing agents, although environmentally attractive, frequently produced nanoparticles with broad size distribution, morphological variability, limited reproducibility, contamination risks, and poor scalability, thereby compromising material performance. To overcome these constraints, we report a colloidal-engineering driven strategy employing synthetic hydrophilic spacer (s)-containing cationic gemini surfactants (g1-g3; alkyl tails, $m = 12$ to 16) as efficient surface-stabilizing agents for the chemical-reduction synthesis of lead (II) sulfide nanoparticles (PbS-g1 to PbS-g3). The hydrophilic s provides a flexible molecular framework that promotes control nucleation, effective surface passivation and enhanced surface passivation, and modulation of the structural and interfacial properties of PbS NPs. Strong gemini-PbS interactions were confirmed through EDX, FT-IR, XRD, and Raman analyses, indicating effective coordination of the gemini's m with the PbS surface. Morphological and thermal analyses (TEM, DLS, TGA) revealed uniformly dispersed spherical nanoparticles (~ 5 - 10 nm) with good thermal stability, except for PbS-g1, while, zeta (ζ)-potential measurements indicated stable positively charged colloidal systems. Optical investigations, using UV–vis and PL spectroscopy, revealed enlarged optical band gaps (E_g) and reduced surface defect states, consistent with quantum confinement and efficient surface passivation. Biological studies demonstrated that gemini-stabilized PbS NPs exhibited suppressed antibacterial and anti-fungal (agar-disc/agar-well diffusion) activity, against *S. aureus*, *E. coli*, *A. niger*, and *C. albicans*, respectively. Collectively, these results establish hydrophilic spacer-based cationic gemini surfactants, as a versatile surface-stabilizers capable of simultaneously tuning structure, optical, colloidal and biological properties in PbS NPs, providing a sustainable platform for next-generation colloidal engineering of PbS and related nanomaterials.

Effect of Controlled Shock Waves on the Structural, Optical and Dielectric Characteristics of Glycine Doped Magnesium Sulfate Single Crystal

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Abstract

The single crystals of glycine-doped magnesium sulfate (GMS) were grown by the slow evaporation solution growth technique. The grown single crystal is subjected to successive acoustic shock-wave loading to study shock-induced defect engineering. PXRD results reveal shock-induced lattice distortion and structural reorganization while preserving the fundamental orthorhombic crystalline framework of GMS. The high optical transparency was revealed by UV-visible absorption spectroscopy. The Raman analysis exhibited the characteristic $V_1(\text{SO}_4^{2-})$ vibrational band at 985 cm^{-1} , confirming the preservation of the sulfate tetrahedral framework. The photoluminescence study shows the emission at 417 nm. The PL intensity increases with shock pulse. The dielectric studies revealed low dielectric loss and good dielectric stability. The chemical etching study showed controlled defect evolution without significant degradation of the surface. These results together indicate that acoustic shock-wave loading is an effective post-growth defect-engineering approach for tailoring the multifunctional properties of GMS crystals non-linear optical applications.

Keywords: Glycine-doped magnesium sulfate; Acoustic shock-wave loading; Defect engineering; Structure-property relationship; Raman spectroscopy; Photoluminescence.

Recent developments in supercapacitor electrode materials: design, performance, and future perspectives

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Abstract

Supercapacitors have gained massive attention as next-generation energy storage devices because of their high-power density, long cycle life, fast charge–discharge rate, and good environmental sustainability. Their role in energy storage and harvesting is crucial, specifically in advanced portable electronic devices. This review presents a comprehensive overview of the recent developments in supercapacitor research by covering the design of electrode materials and the advancements in developing novel materials. The recent developments in the fields of electric double-layer capacitors, hybrid supercapacitors, and pseudocapacitors, with a particular focus on their electrode materials, are also discussed. The major focus is on two-dimensional (2D) materials including carbon aerogels, carbon foams, carbide-derived carbons, graphenes, CNTs, activated carbons, TMDs, h-BN, MXenes, and carbon nitrides, which exhibit excellent electrochemical properties for supercapacitor applications. Transition metal oxides such as RuO_2 , ZnO , NiO , Co_3O_4 , MnO_2 , $\text{Fe}_2\text{O}_3/\text{Fe}_3\text{O}_4$ and V_2O_5 are also enticing electrode materials for supercapacitors owing to their excellent redox behavior and high energy density. Finally, the challenges and future perspectives are discussed, along with providing potential strategies for electrode performance enhancements.

Key words: Supercapacitors, Energy storage, electrode.

A Sustainable Nano-catalyst for the Production of Biodiesel Using Fat Derived from Chicken Processing Waste

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Abstract

Recent research strives to find a substitute for conventional transportation fuels to address the growing energy demand. Biodiesel is known for its eco-friendliness, non-toxic nature, sustainability and biodegradability. The feedstock determines the cost of the biodiesel and catalyst used for its production. This study employs a low-cost feedstock and a recoverable and reusable catalyst to reduce the overall cost. Fat from chicken processing sludge was used in biodiesel production using methanol and a recoverable and reusable nano-catalyst (CaO/Fe₃O₄/Cs₂O) via transesterification reaction. Chemical co-precipitation and wetness impregnation methods were employed to prepare the magnetic nano-catalyst. Further, it was characterized by X-Ray Diffraction (XRD), Scanning Electron Microscope (SEM), and Fourier Transform Infrared Spectroscopy (FTIR) to understand its chemical and physical characteristics. Vibrating Sample Magnetometer (VSM) analysis is done to analyze magnetic properties. The catalyst performance was evaluated by transesterification reaction, which resulted in 98.3 % conversion under optimum conditions: catalyst loading of 8 wt.%, methanol to fat molar ratio of 21:1, 65 °C of reaction temperature, and 240 min of reaction time with 450 rpm stirring rate. It is found that the fuel properties of the biodiesel were in line with the ASTM D6751 standards. Furthermore, an investigation was conducted on the kinetics ($E_a = 110.82 \text{ kJ mol}^{-1}$; $k = 0.028 \text{ min}^{-1}$ at 333 K) and reusability of the catalyst. It demonstrated that the catalyst could be effectively recycled up to five times while maintaining a conversion of over 92 % in each successive cycle.

Keywords: Reusable nano-catalyst, co-precipitation, wetness impregnation method, transesterification, low-cost feedstock, biodegradable.

Emerging Energy Storage Materials for Sustainable Energy Systems: A Review of Recent Developments and Future Trends

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Abstract

The accelerating global shift toward renewable power generation has made energy storage the pivotal bottleneck standing between intermittent supply and reliable demand. This review synthesizes recent developments in materials for electrochemical, capacitive, thermal, chemical, and mechanical energy storage, with particular emphasis on advanced electrode, electrolyte, and nanostructured materials developed between 2022 and 2026. Cathode chemistries (LiFePO₄, NMC, NCA, sulfur), anode materials (graphite, silicon, hard carbon, lithium metal), and solid, polymer, and liquid electrolytes are examined alongside emerging sodium, potassium, zinc, magnesium, and aluminium-ion chemistries that reduce dependence on scarce lithium and cobalt resources. Supercapacitor electrodes based on carbons, transition-metal oxides, and conducting polymers are compared with battery materials on the basis of energy density, power density, and cycle life. A dedicated treatment of emerging nanomaterials-graphene, carbon nanotubes, MXenes, metal-organic frameworks, covalent-organic frameworks, transition-metal dichalcogenides, and heterostructures-links nanoscale architecture to ion-transport kinetics and electrochemical performance. A distinguishing feature of this review is its emphasis on sustainable and bio-derived materials, including biomass- and agricultural-waste-derived carbons, green synthesis routes, and recycled battery materials, framed within a circular-economy perspective. Principal material-modification strategies (doping, defect engineering, nanostructuring, heterostructure and core-shell design, and composite formation) are critically discussed together with the persistent challenges of cycle-life degradation, dendrite formation, thermal runaway, critical-raw-material dependence, and the gap between laboratory and commercial performance. The growing role of artificial intelligence and machine learning in materials discovery, degradation prediction, and digital-twin-based system optimization is also surveyed. The review concludes by identifying key research gaps and future directions toward energy-dense, safe, low-cost, and environmentally benign storage materials for next-generation sustainable energy systems.

Keywords: energy storage materials; lithium-ion batteries; sodium-ion batteries; supercapacitors; nanomaterials; biomass-derived carbon; solid-state electrolytes; machine learning; sustainability; circular economy

Unlocking the catalytic potency of varied NiFe₂O₄ magnetic nanoparticles for the sustainable synthesis of tri- and tetra-substituted imidazoles

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Abstract

A practical and eco-friendly catalytic system based on NiFe₂O₄ magnetic nanoparticles has been devised for the fast and high-yielding preparation of diverse 2,4,5-trisubstituted and 1,2,4,5-tetrasubstituted imidazoles using methanol as the solvent. The method is notable for its simplicity, broad substrate compatibility, and clean reaction profiles. It offers several benefits over earlier protocols: shorter reaction durations, superior yields, uncomplicated procedures, easy work-up, and the ability to recover and reuse the catalyst magnetically. The structural and morphological features of the synthesized NiFe₂O₄ nanoparticles were investigated using FTIR, XRD, EDX, SEM, and TEM.

Keywords: Imidazole, Methanol, NiFe₂O₄ nanoparticles, magnetic

Chemical and Compositional Effects on the Magnetic, Dielectric and Thermal Behaviour of Poly(o-phenylenediamine)/ CrSrFe₂O₄ Nanocomposites

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Abstract

This work investigates the synthesis and properties of CrSrFe₂O₄/poly(o-phenylenediamine) (CrSrFe₂O₄/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 CrSrFe₂O₄ 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 CrSrFe₂O₄ 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 CrSrFe₂O₄/PoPD nanocomposites have significant potential in multifunctional material design for next-generation technologies.

Keywords: PoPD, CrSrFe₂O₄, PXRD, SEM, TEM, Magnetic studies, Electrical studies

Unravelling the Optoelectronic Properties of the Antiperovskite Zn_3PN : A First-Principles Study

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Abstract

The search for efficient and earth-abundant materials for photovoltaic and optoelectronic applications has stimulated considerable interest in antiperovskite compounds. In this work, we investigate the structural, electronic, optical, and charge-carrier properties of Zn_3PN , a theoretically predicted antiperovskite with a $P2_1ma$ orthorhombic crystal structure, using first-principles calculations within density functional theory. Zn_3PN is found to be an indirect-bandgap semiconductor with highly dispersive conduction-band edges. Although the material exhibits an indirect band gap, its optical and charge-carrier properties require detailed investigation to scrutinize its potential for optoelectronic and photovoltaic applications. Accordingly, the frequency-dependent dielectric function, absorption coefficient, reflectivity, and related optical properties are systematically evaluated to understand its interaction with electromagnetic radiation. In addition, the charge-carrier properties are investigated to assess the carrier transport characteristics of Zn_3PN . The combined analysis of the electronic structure, optical response, and charge-carrier properties provides a comprehensive understanding of the material's fundamental characteristics and its potential suitability for optoelectronic applications. The present study provides theoretical insights into Zn_3PN and establishes a basis for further experimental investigations of this antiperovskite compound.

Keywords: Antiperovskite, First-Principles Calculations, Optoelectronic Properties

DFT study of 1, 2-(η^5 -C₅H₅)₂M₂B₄H₆ (M = Co, Rh, Ir) and BH activation using F, Cl, Br and I

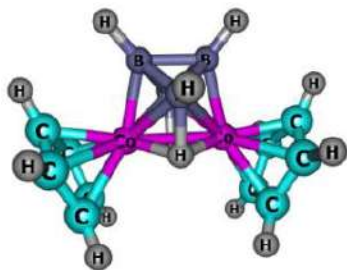
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Abstract

Metallaboranes playing main role in both medical and industrial fields (BNCT, *anti*-HIV, BH activation, hydrogen storage device, solid state electrolytes, optoelectric materials and etc).[1-6] It is a hybrid of borane chemistry and metal chemistry, this chemistry is termed as inorganometallic chemistry proposed by T. P. Fehlner.[1] Metallaboranes has the ability to form metal rich and boron rich clusters. Most of the dimetallaboranes has both bridging and terminal hydrogens but the bridging hydrogen can form (μ_2 -H) and (μ_3 -H) bridging multiplicity with boranes and metals. Here, we have investigate using geometry, NMR, FMO, MBO, WBO and ELF analysis of 1, 2-(η^5 -C₅H₅)₂M₂B₄H₆ (M = Co, Rh, Ir), the μ_3 connected bridging hydrogens contained six vertex '*closo*' dimetallaboranes at BP86/Def2-TZVP/ZORA/D4 level. DFT has been proved considerable success in structural characterization and modeling.[4-6] First proposed cluster of this class is 1, 2-(η^5 -C₅H₅)₂Co₂B₄H₆ by R. N. Grimes et al.[2, 3] The bridging hydrogen contained '*closo*' polyhedral metallaboranes has unique electronic structure and structural features. So, we have investigated these clusters using B-H activation (F, Cl, Br and I) using various probabilities and checking the antipodal effects and M-M (M-metal) interactions. The substitution at the antipodal vertices improves the strength of the M-M bond and decreases *antipodal* effect between the metal and antipodal boron vertices at the top.[4]

Keywords: Metallaborane, bond order, antipodal effect, (μ_3 -H) bridging multiplicity



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Quantum Dots: A Promising Nanomaterial For Advanced Applications

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Abstract

Quantum dots (QDs) are zero-dimensional nanomaterials possessing unique sizedependent optical and electronic properties arising from quantum confinement effects. Their tunable emission, broad absorption, high photoluminescence, and surface functionalization ability make them attractive materials for advanced technological and biomedical applications. Recent experimental studies have demonstrated the potential of QDs in fluorescence imaging, sensing, optoelectronics, and energy-related applications. For example, PDMS-coated CdTe QDs have demonstrated size-dependent multi colour fluorescence for simultaneous imaging of cellular organelles, highlighting their potential as optical probes in biomedical research. QDbased materials have also been investigated for sensitive detection of chemical and biological analytes through their distinctive optical and electrochemical responses. In addition, the tunable electronic structure and strong light–matter interactions of QDs provide opportunities for applications in light-emitting devices, photovoltaics, and photocatalysis. This work highlights the fundamental properties, synthesis approaches, and characterization of QDs, with particular emphasis on their emerging applications. The influence of particle size, composition, surface chemistry, and quantum confinement on their functional performance is also discussed. The challenges associated with toxicity, stability, reproducibility, and large-scale synthesis are considered, along with future prospects for developing safer and multifunctional QD-based materials.

Keywords: Quantum dots; Nanomaterials; Quantum confinement; Optical properties; Bioimaging; Photocatalysis; Photovoltaics

Rational Design of a Spherical Ternary NiCoMn@Ionic Liquid Nanocomposite for Enhanced Electrochemical Vanillin Sensing: Structure–Property Correlations

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Abstract

The rational design of high-performance nanostructured electrochemical interfaces is essential for the sensitive and selective detection of food-related bioactive compounds. In the present study, a spherical ternary NiCoMn metal–organic framework (MOF) was rationally engineered and integrated with the ionic liquid [BMIM][MeSO₄] to develop a highly efficient GCE/IL/NiCoMn-MOF electrochemical sensor for vanillin detection. The sensing performance of the ternary NiCoMn-MOF was systematically evaluated in comparison with Co-MOF and NiCo-MOF, demonstrating the synergistic contribution of the three metal centers toward improved electrochemical activity. The synthesized nanomaterials were comprehensively characterized using scanning electron microscopy (SEM), energy-dispersive X-ray (EDX) elemental mapping, X-ray diffraction (XRD), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and thermogravimetric analysis (TGA), confirming their morphology, elemental composition, structural characteristics, surface chemical states, and thermal stability. Cyclic voltammetry (CV) revealed a substantially enhanced electroactive surface area for the ternary NiCoMn-MOF-modified electrode, approximately eight times higher than that of the bare GCE, while electrochemical impedance spectroscopy (EIS) confirmed the improved charge-transfer characteristics of the ionic-liquid-integrated interface. The optimized GCE/IL/NiCoMn-MOF platform exhibited a pronounced oxidative response toward vanillin, a naturally occurring phenolic aldehyde predominantly obtained from *Vanilla planifolia* pods. The electrochemical behaviour of vanillin was systematically investigated by optimizing experimental parameters including pH and scan rate. The well-defined oxidation response was further explored to elucidate the electrochemical transformation of vanillin. Square-wave voltammetry (SWV) enabled highly sensitive quantitative determination of vanillin, affording a coefficient of determination (R^2) of 0.998, a reported limit of detection (LOD) of 26 nM, and a limit of quantification (LOQ) of 79 nM. The sensor exhibited a sensitivity of 10.55 $\mu\text{A } \mu\text{M}^{-1} \text{ cm}^{-2}$ and excellent analytical recovery in real samples, ranging from 98–102%. Furthermore, the developed sensor demonstrated very good repeatability, reproducibility, operational stability, and resistance to interference from potentially competing compounds present in natural vanilla extracts.

Overall, the synergistic integration of the ternary NiCoMn-MOF with an ionic liquid provides an efficient electrochemical platform for vanillin determination, highlighting the importance of multimetallic MOF engineering in improving electrode surface area, charge-transfer characteristics, and analytical performance. To the best of our knowledge, this study represents a novel application of a ternary NiCoMn-MOF-based electrochemical platform for vanillin sensing and provides a promising strategy for sensitive analysis of vanillin in food-related samples.

Keywords: NiCoMn-MOF; ternary metal–organic framework; ionic liquid; electrochemical sensor; vanillin; square-wave voltammetry; food analysis; electroactive surface area; nanocomposite.

Geometrical and Electronic Structure, Stability, Bonding and Spectroscopic Studies on Metanil Yellow and its Derivatives – A DFT Study

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Abstract

Food is adulterated commonly in countries like India, to increase the quantity and make more profit. An adulterant is a chemical substance which should not be contained within other substances (e.g. food, beverages, and fuels) for legal or other reasons. The addition of adulterants is called adulteration. Food fraud was recently defined as a collective term that encompasses the deliberate substitution, addition, tampering or misrepresentation of food, food ingredients or food packaging, or false or misleading statements made about a product for economic gain.¹ Turmeric, dals and pulses such as moong or channa are adulterated with Metanil Yellow (Sodium 3-[(4-anilinophenyl)diazenyl]benzenesulfonate) and Kesari Dal to enhance the yellow colour of a food substance. These adulterants are highly carcinogenic and if consumed over a continuous period of time it can cause liver, kidney and heart problems, diarrhea, giddiness, severe joint pains and stomach disorders. Further the addition of starch greatly reduces the nutritional value of the ingredient.^{2,3} The important structural features and biological implications of the adulterant Metanil Yellow (Sodium 3-[(4-anilinophenyl)diazenyl]benzenesulfonate) has been studied using the molecular orbital calculations like semi-empirical methods and density functional theory (DFT) methods. Computational methods have already been proved to be a promising tool to study the structural aspects and reactivity of the biologically important molecules. The intrinsic electrophilic and nucleophilic centers of the molecule and their interactions with the selected proteins are predicted using the computational tools. The interesting results obtained from the calculations will be presented.

OP-EN-55

**SYNTHESIS, GROWTH AND CHARACTERIZATION OF NLO
ACTIVE ORGANIC CRYSTAL**

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Abstract

Nonlinear optical (NLO) materials play a vital role in modern photonic and optoelectronic technologies due to their applications in optical communication, signal processing, data storage, and laser-based devices. Among various NLO materials, organic crystals have gained significant attention because of their superior optical nonlinearity, structural flexibility, and ease of molecular tailoring compared to inorganic counterparts. In this work, the synthesis, crystal growth, and characterization of NLO-active organic crystals based on Schiff base derivatives are reported. Schiff base compounds, formed through the condensation of substituted amines with substituted aldehydes, exhibit strong donor–acceptor interactions and extended π -electron conjugation, which are essential for enhanced NLO response. The synthesized compounds were structurally confirmed using elemental analysis and Fourier Transform Infrared (FTIR) spectroscopy. Single crystals suitable for optical applications were successfully grown, and their crystalline nature was confirmed by single crystal X-ray diffraction (SCXRD) studies. The optical properties of the grown crystals were systematically investigated to evaluate their suitability for NLO applications. The results demonstrate that the synthesized Schiff base organic crystals exhibit promising nonlinear optical behaviour, making them potential candidates for applications such as second harmonic generation, frequency conversion, optical modulation, and photonic devices.

Anion Exchange Membrane for Energy Devices

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Abstract

The global shift towards clean and sustainable energy has intensified interest in hydrogen-fuelled technologies, particularly fuel cells. Among these, Proton Exchange Membrane Fuel Cells (PEMFCs) dominate the market due to their compact design and high power density. However, PEMFCs operate under acidic conditions, requiring expensive noble metal catalysts like platinum, and depend on costly perfluorinated membranes for ionic conduction. These factors significantly increase the overall system cost, limiting their scalability for widespread adoption. In this context, Anion Exchange Membrane Fuel Cells (AEMFCs) have emerged as a promising alternative, offering several advantages. Operating in alkaline conditions, AEMFCs enable the use of non-precious metal catalysts, drastically reducing material costs while maintaining competitive performance. However, challenges such as membrane stability, ionic conductivity, and mechanical integrity must be overcome to position AEM technology as a viable competitor to PEMFCs. This study focuses on the development of a polyvinyl alcohol (PVA)-based Anion Exchange Membrane (AEM) tailored for fuel cell applications. PVA was selected due to its excellent film-forming ability, chemical stability, and affordability. The membrane was synthesized by chemically modifying PVA with quaternary ammonium groups, enhancing its anion conductivity and alkaline stability. Comprehensive characterization studies were carried out to assess the membrane's suitability for AEMFCs. Ion exchange capacity (IEC) measurements revealed a high concentration of functional groups, ensuring superior anion conductivity. Water uptake and swelling behavior were optimized to maintain membrane integrity under hydrated operating conditions. Thermal and mechanical analyses confirmed the material's robustness, while chemical stability tests demonstrated excellent resistance to degradation in alkaline environments.

KeyWords: Polyvinyl alcohol, Fuel cell, AnionicExchangeMembrane, Conductivity

Sustainable Fabrication of NiCo₂O₄ Nanoparticles via *Pedalium murex* Extract for High-Performance Supercapacitor Electrodes

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Abstract

Green synthesis has emerged as a sustainable and environmentally friendly approach to nanomaterial fabrication, offering the potential to minimize the use of hazardous chemicals and energy-intensive processing associated with conventional synthesis methods. In this study, a novel eco-friendly approach was employed to synthesize nickel cobaltite (NiCo₂O₄) nanoparticles using *Pedalium murex* extract as a natural bioactive agent, facilitating nanoparticle formation and stabilization. The X-ray diffraction (XRD) pattern confirmed the successful formation of a cubic spinel structure with nanoscale crystallites. Field-emission scanning electron microscopy (FE-SEM) and energy-dispersive X-ray spectroscopy (EDX) analyses provided information regarding the morphology and elemental composition of the synthesized material. The electrochemical performance of the as-prepared NiCo₂O₄ nanostructures was evaluated using cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS). The electrode exhibited a maximum specific capacitance of 465 F g⁻¹ at a current density of 0.8 mA cm⁻² in 3 M KOH electrolyte, together with 88.8 % capacitance retention after 2,600 charge–discharge cycles. These findings highlight the potential of spinel NiCo₂O₄ nanostructures as electrode materials for sustainable supercapacitor applications.

Keywords: Green synthesis, *Pedalium murex*, spinel NiCo₂O₄, Supercapacitor applications.

Microwave-Hydrothermal Synthesised In-Doped ZnO/rGO as a High-Performance Supercapacitor Electrode

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Abstract

To address escalating global energy demands, developing advanced materials with superior electrochemical performance for next-generation energy storage is critical. In this work, indium doping was strategically utilized to tailor the capacitive properties of pristine ZnO. Utilizing a rapid microwave-assisted hydrothermal method, a diverse suite of samples was synthesised, such as Pure ZnO, indium-doped ZnO nanoparticles with varying dopant concentrations (3, 5, and 7 wt%), and an optimized indium-doped ZnO composite anchored on reduced graphene oxide (rGO). The structural, morphological, and elemental signatures of the prepared materials were comprehensively evaluated via XRD, FTIR, BET, Raman spectroscopy, XPS, FESEM-EDX, and HRTEM. Electrochemical evaluations performed in a three-electrode configuration revealed that the optimized composite electrode (designated as ZING) achieved an outstanding specific capacitance of 695 F g⁻¹. Furthermore, the electrode exhibited exceptional durability, retaining 84% of its initial capacitance after a rigorous 10,000 cycle stability test, highlighting its potential for high-performance supercapacitor applications.

Keywords: - In-doped ZnO/rGO, Microwave-Hydrothermal synthesis, Electrochemical energy storage, Pseudocapacitors, cyclic stability.

Improved Durability of MAPbI₃ Hybrid Perovskite Solar Cells with 2-Aminobenzothiazole

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Abstract:

The long-term stability of MAPbI₃ perovskite remains limited when exposed to light, heat, and humidity, posing a major challenge to commercialization. Its degradation and the hindrance of non-radiative charge recombination, crucial for improving the stability and efficiency of photovoltaic devices, are driven by trap states and surface imperfections at the interfaces between the perovskite and the ETL. In this investigation, we remedied surface defects by applying 2-aminobenzothiazole, which activates the heteroatoms of sulfur and nitrogen and the amine functional group to passivate defects. The systematic investigation focused on hydrogen-bond formation between N—H—I and coordination between uncoordinated Pb²⁺ ions and the heteroatoms of sulfur and nitrogen. The optimized passivating material concentration of 2 mg/ml IPA achieved a high photovoltaic efficiency of 21.5%, with improvements in V_{oc} and FF, surpassing the pristine MAPbI₃ PCE of 19.4%. Durability tests showed that the 2-ABT-integrated device performed better than the unmodified MAPbI₃ device, retaining 87% of its PCE after 500 hours in nitrogen.

Keywords: Perovskite solar cells, stability, defects, and recombination.

OP-EN-60

Influence of Barium Doping on the Frequency-Dependent Dielectric Properties of Biogenically Synthesized Cobalt Ferrite Nanoparticles

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Abstract

Biogenic synthetic route was employed for the preparation of barium doped cobalt ferrite (Co_{1-x} Ba_x Fe₂O₄) nanoparticles. Different concentrations of barium were added as a dopant in cobalt ferrites CoFe₂O₄ nanoparticles to get (Co_{1-x} Ba_x Fe₂O₄) where x = 0, 0.25, 0.50, 0.75 and 1.0 moles. X-ray diffraction (XRD) spectroscopy was employed for the analysis of crystallographic structure and Debye-Scherrer formula was employed for the determination of average crystallite size. The morphological study and size calculation of Co_{1-x} Ba_x Fe₂O₄ nanoparticles were carried out by using scanning electron microscopy (SEM). Energy dispersive X-ray (EDX) spectroscopy was used for the elemental analysis of the synthesised nanoparticles. The vibrational modes of different atoms present in these nanoparticles were investigated using Fourier transform infrared (FTIR) spectroscopy. The dielectric parameters such as capacitance, real and imaginary parts of dielectric constant, loss tangent and AC-conductivity were inspected using LCR meter. Significant improvement in charge storage and transport properties were achieved with the doping of barium in CoFe₂O₄ nanoparticles.

Keywords: Barium doped cobalt ferrite nanoparticles, XRD, SEM with EDX, capacitance, dielectric constant, charge storage

Corrosion Inhibition of Mild Steel in 0.5 M H₂SO₄ using *Tecoma stans* flower Extract: Electrochemical and Adsorption Studies

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Abstract

The present study investigates the corrosion inhibition efficiency of *Tecoma stans* flower extract (TSFE) on mild steel in 0.5 M H₂SO₄ solution. The extract was prepared using the Soxhlet extraction method and evaluated as a green corrosion inhibitor. The effects of inhibitor concentration and temperature on the corrosion behaviour of mild steel were investigated. The results showed that the inhibition efficiency increased with increasing TSFE concentration, reaching a maximum of 94.25%. Polarization studies indicated that TSFE acts as a mixed-type corrosion inhibitor. The polarization results revealed that the addition of TSFE increased the polarization resistance (R_p) and decreased the corrosion current density (I_{corr}), indicating enhanced corrosion resistance of mild steel in 0.5 M H₂SO₄. Electrochemical impedance spectroscopy (EIS) further demonstrated an increase in charge transfer resistance (R_{ct}) and a decrease in double-layer capacitance (C_{dl}) in the presence of TSFE, confirming its protective effect on the mild steel surface. The adsorption behaviour of TSFE followed the Langmuir adsorption isotherm. The open-circuit potential (OCP) values of the inhibited systems were shifted towards more negative potentials compared with the uninhibited system. FTIR analysis of the TSFE and the protective film obtained from the mild steel surface after immersion revealed characteristic functional groups, with slight shifts in the corresponding absorption bands, suggesting their involvement in the interaction with the metal surface. AFM analysis showed that the mild steel specimen immersed in TSFE exhibited comparatively less surface deterioration than the specimen immersed in 0.5 M H₂SO₄ alone. The electrochemical and weight-loss measurements showed good agreement in the corrosion inhibition performance. Overall, *Tecoma stans* leaf extract can be considered a promising, eco-friendly, low-cost, and sustainable inhibitor for the corrosion of mild steel in 0.5 M H₂SO₄.

Key words: Corrosion, *Tecoma stans*, mild steel, 0.5 M H₂SO₄

Synergistic Charge Storage in Zinc–Cerium Bimetallic Metal–Organic Framework/Graphene Oxide Composites for High-Performance Supercapacitors

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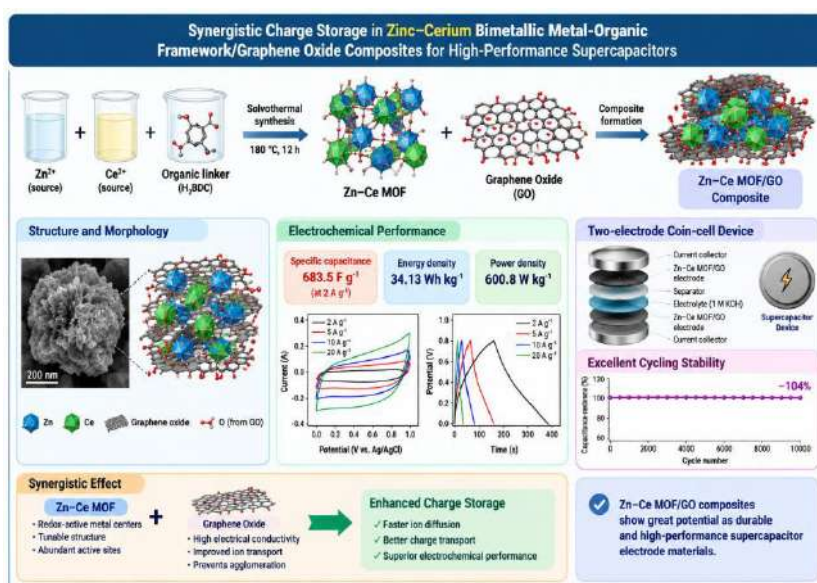
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Abstract

Bimetallic metal–organic frameworks (BMOFs) have emerged as promising electrode materials for electrochemical energy storage owing to their tunable structures, abundant active sites, and redox-active metal centers. However, their limited electrical conductivity and restricted ion transport can hinder their practical application in supercapacitors. In this study, a zinc–cerium bimetallic metal–organic framework (Zn–Ce MOF) was synthesized and integrated with graphene oxide (GO) to develop a Zn–Ce MOF/GO composite electrode for enhanced electrochemical energy storage. The incorporation of GO provides a conductive network that facilitates charge transport, improves electrolyte ion accessibility, and suppresses particle agglomeration. The Zn–Ce MOF/GO electrode demonstrates enhanced electrochemical performance in 1 M KOH electrolyte, delivering a specific capacitance of 683.5 F g^{-1} at 2 A g^{-1} , together with an energy density of 34.13 Wh kg^{-1} and a power density of 600.8 W kg^{-1} . Furthermore, a two-electrode coin-cell device fabricated using the Zn–Ce MOF/GO composite exhibits excellent cycling stability, maintaining approximately 104% of its initial capacitance after 10,000 charge–discharge cycles, which can be associated with electrochemical activation during the initial cycling process. The enhanced charge-storage behavior is attributed to the synergistic interaction between the redox-active Zn–Ce bimetallic framework and the GO network, promoting efficient ion diffusion and charge transport. These findings demonstrate the potential of Zn–Ce MOF/GO composites as electrode materials for durable and high-performance supercapacitor devices.

The Zn–Ce MOF/GO composite electrode demonstrates enhanced electrochemical performance in 1 M KOH electrolyte, delivering a specific capacitance of 683.5 F g^{-1} at 2 A g^{-1} , together with an energy density of 34.13 Wh kg^{-1} and a power density of 600.8 W kg^{-1} . Furthermore, a two-electrode coin-cell device fabricated using the Zn–Ce MOF/GO composite exhibits excellent cycling stability, maintaining approximately 104% of its initial capacitance after 10,000 charge–discharge cycles, which can be associated with electrochemical activation during the initial cycling process. The enhanced charge-storage behavior is attributed to the synergistic interaction between the redox-active Zn–Ce bimetallic framework and the GO network, promoting efficient ion diffusion and charge transport. These findings demonstrate the potential of Zn–Ce MOF/GO composites as electrode materials for durable and high-performance supercapacitor devices.

Key words: Bimetallic metal–organic frameworks (BMOFs), composite, cycling stability, supercapacitor.



MXene and Si@C Composites with Spinel Mixed Metal Oxides for High-Performance Supercapacitors

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Abstract

The development of high-performance electrode materials with enhanced electrical conductivity, rapid ion transport, and structural stability is essential for advancing next-generation supercapacitors. In this study, a synergistic composite architecture comprising MXene, Si@C, and spinel mixed metal oxides is proposed for efficient electrochemical energy storage. The Si@C component provides a stable carbon-confined silicon framework, while the two-dimensional MXene sheets offer highly conductive pathways and interconnected interfaces for efficient electron transport. Incorporation of spinel mixed metal oxides introduces abundant redox-active sites and enhances the faradaic contribution of the composite electrode. The rational integration of these components is expected to establish a hierarchical conductive network with improved electrode–electrolyte interaction and shortened ion diffusion pathways. The synthesized composites are systematically investigated using structural, morphological, surface, and spectroscopic characterization techniques, including X-ray diffraction, Raman spectroscopy, FTIR, electron microscopy, BET surface-area analysis, and X-ray photoelectron spectroscopy. Their electrochemical behavior is evaluated through cyclic voltammetry, galvanostatic charge–discharge, electrochemical impedance spectroscopy, rate capability, and cycling stability measurements. The synergistic interaction among MXene, Si@C, and spinel mixed metal oxide is investigated to elucidate the relationship between interfacial structure and charge-storage mechanism. This work provides a versatile materials-design strategy for developing multifunctional MXene/Si@C-based composite electrodes for advanced supercapacitor applications.

Keywords: MXene, Silicon, Metal Oxides, Supercapacitors.

From Machine Learning to Quantum Chemistry: An Integrated Strategy for KRAS G12D Inhibitor Discovery

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Abstract

KRAS G12D is a frequent oncogenic mutation associated with pancreatic ductal adenocarcinoma and several other cancers. Unlike KRAS G12C, the G12D variant lacks a reactive cysteine and therefore requires non-covalent targeting of the switch-II (S-II) pocket. The limited availability of clinically advanced KRAS G12D inhibitors highlights the need for structurally diverse candidate molecules. In this study, a multi-step computational workflow was applied to identify and prioritize potential KRAS G12D inhibitors. A dataset of 592 standardized bioactivity records was obtained from ChEMBL and used to develop fingerprint-based machine-learning models. A Random Forest classifier differentiated active and inactive compounds with a held-out ROC-AUC of 0.880, whereas continuous pIC₅₀ regression showed limited predictive performance (cross-validated R² approximately 0.07–0.09). Bemis-Murcko scaffold analysis and BRICS-based molecular generation were followed by molecular docking against KRAS G12D (PDB 9E5F). Seven structurally diverse compounds showed better docking scores than the reference compound CHEMBL3577124 (−8.3 kcal/mol). CHEMBL5917657 showed the highest predicted binding score (−12.1 kcal/mol), but its larger size, higher lipophilicity, lower predicted solubility, and greater synthetic complexity limited its overall prioritization. KRAS_CC_0030 and KRAS_C4_18 showed favorable docking profiles together with predicted physicochemical properties, synthetic accessibility, and molecular flexibility compatible with further evaluation. Density functional theory, CABS-flex analysis, and ADME prediction provided complementary structural and physicochemical information. The results demonstrate the utility of integrating molecular modelling, quantum chemical analysis, flexibility assessment, and computational ADME evaluation for prioritizing KRAS G12D inhibitor candidates for experimental validation.

Keywords: KRAS G12D, molecular docking, quantum chemistry, drug discovery, computational screening

Engineering a g-C₃N₄/Fe-V Mixed oxide/PANI Hybrid Electrode for High-Performance Supercapacitor Applications

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Abstract

The development of high-performance supercapacitors needs the rational integration of an electrically conductive framework, such as redox-active components and a structurally stable matrix, to maximise the charge storage kinetics. Graphitic Carbon Nitride g-C₃N₄ is a carbon based compound containing nitrogen, which helps the carbon framework increase polarity and structural stability. Iron oxides can undergo surface redox reactions and contribute to the pseudo capacitance, providing electrochemically active sites and also improving charge storage capacity. Vanadium exhibits various oxidation states such as V²⁺, V³⁺, V⁴⁺, V⁵⁺, which undergo multiple reversible redox reactions, improving capacitance and providing additional charge storage capacity. Hence, g-C₃N₄ has been incorporated with iron and vanadium oxides to increase the electrochemical performance. The g-C₃N₄/FeV mixed oxide composite has been prepared by the hydrothermal process. Further, it is incorporated with conductive polyaniline through in situ oxidative polymerization. The prepared materials were characterized using appropriate techniques such as X-ray diffraction (XRD). Its electrochemical performance was evaluated using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). The resulting composite provides a synergistic impact of double-layer capacitance, charge transfer kinetics, and overall electrochemical energy storage.

Keywords: Supercapacitor, g-C₃N₄, polyaniline, hybrid composite, pseudocapacitance

Hydrothermal Synthesis of Chromium (II) Sulphate Doped Cuprous (I) Oxide for Optical Applications

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Abstract

Cuprous oxide (Cu_2O) nanocomposites doped with chromium sulphate (CrSO_4) were created using a straight forward low-cost and chemical method. The goal of the study was to improve the properties of pure Cu_2O such as structural, optical, and electro-chemical by synthesizing Cu_2O in four different methods using CrSO_4 as a dopant. The Cu_2O characterized at each stage of synthesis in relation to the morphology size, shape, etc., crystallinity, The UV-VIS spectrophotometry studies showed a shift in absorption edge which is an indicative that the band gap changed as a result of the incorporation of chromium into the Cu_2O crystals. The FTIR spectra demonstrated that the dopant molecules have been successfully incorporated into the Cu_2O crystalline structure. XRD demonstrated the presence of crystalline peaks of cubic Cu_2O and the cubic crystalline structure was not affected. The SEM photographs show that the majority of the particles are quasi-spherical shape and the materials are at the Nano scale. Cyclic voltammetry demonstrated that the electrochemical characteristics of Cu_2O doped with CrSO_4 have improved compared to those exhibited by undoped Cu_2O . The GCD experiments provided evidence that the capacitance for the doped samples was much greater and much better cyclic reversibility and excellent cycling stability, thus showing that these materials hold great promise as potential energy storage materials.

Keywords: Cyclic voltammetry, cubic crystalline structure, Galvanostatic charge-discharge curves, XRD, SEM, etc.

Growth of thin films of Cu₃N at room temperature without any bias, suitable for use in flexible electronics

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Abstract:

This research explores the synthesis of highly (100) oriented nanocrystalline Copper Nitride (Cu₃N) thin films at room temperature using reactive RF magnetron sputtering. Importantly, the process does not involve pre- or post-annealing steps, nor does it use substrate biasing. The study examines how the structural development and mechanical properties of the films are related using X-ray diffraction (XRD), scanning electron microscopy (SEM), and atomic force microscopy (AFM). XRD results show that the films have a nanocrystalline structure with a notable micro-strain of 12.8×10^{-3} and lattice expansion of 3.87 Å. These features are linked to the high rate of nitrogen species bombardment, which is maintained at 60 sccm. AFM analysis of the surface reveals a very smooth surface with an RMS roughness (S_q) of 1.61 nm and a symmetrical height distribution ($S_{sk} = -0.26$) in the best-performing samples. However, as the thickness of the films increases, the built-up compressive stress causes mechanical instability, resulting in the formation of buckling ridges and heart-shaped spallation features, as seen in SEM images. The high kurtosis ($S_a = 34.6$) in the AFM 3D topography further indicates localized strain-induced vertical growth. This detailed connection between high intrinsic micro-strain and surface morphology offers important information about the growth processes of Cu₃N films, which is essential for developing stable and efficient optoelectronic and smart window applications.

Keywords: Cu₃N thin films, RF Sputtering, without pre and post annealing, without biased sputtering.

Preperation of Gd^{3+} Doped $Ca_9ZnLi(PO_4)_7$ Phosphors for Luminescence Properties

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Abstract

The preparation of $Ca_9ZnLi(PO_4)_7$ phosphor doped with Gd^{3+} increase the understanding of the behaviour of rare earth ions doped in the bulk and nano-sized phosphors. In this investigation solid state reaction method was used at high temperature for the preparation of the Gd^{3+} doped $Ca_9ZnLi(PO_4)_7$ sample material. The investigation of XRD pattern of the sample shows the crystalline size in the nano region of the prepared phosphor. The prepared samples exhibit the properties of Thermoluminescence (TL), and Photoluminescence (PL). The study may be helpful for the development of its applications in the luminescent devices.

Keywords: *Solid State Reaction Method/Luminescence/ XRD / Rare Earth doped phosphor*

Enhanced the Electrocatalytic Water Splitting (HER/OER) Using Novel g-C₃N₄/WO₃/CeO₂ Ternary Nano Composite.

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Abstract

The development of efficient and cost-effective electrocatalysts remains a critical challenge for sustainable hydrogen production. In this work, we report a ternary g-C₃N₄/WO₃/CeO₂ composite synthesized via a wet impregnation method, with CeO₂ nanoparticles and WO₃ nanorods prepared by a simple hydrothermal route. The heterostructure was designed to optimize both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). CeO₂ nanoparticles and WO₃ nanorods were anchored on g-C₃N₄ nanosheets, where WO₃ improved charge mobility, surface reactivity, and catalytic stability under alkaline conditions. X-ray photoelectron spectroscopy (XPS) confirmed strong interfacial interactions and mixed-valence Ce⁴⁺/Ce³⁺ states, facilitating charge transfer and redox activity. The nitrogen-rich framework of g-C₃N₄ accelerated proton transfer during HER, while WO₃ enhanced OER kinetics through improved electron conductivity and active oxygen species generation. This synergistic combination demonstrates a promising pathway toward integrated water-splitting applications using earth-abundant materials.

Keywords: Electrocatalysis, g-C₃N₄, WO₃, CeO₂, Hydrogen Evolution Reaction (HER), Oxygen Evolution Reaction (OER), Sustainable H₂ production.

Pseudocapacitive Behavior of Neodymium-substituted Strontium Cobalt Ferrite Nanoparticles for Energy Storage applications

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Abstract

Neodymium-substituted Strontium Cobalt Ferrite nanoparticle explored as a novel pseudocapacitive material for supercapacitor applications, offering a promising solution for energy storage and conversion devices. Neodymium substitution enhances the electrochemical properties of the material, resulting in improved pseudocapacitive behavior. The nanoparticles exhibit a high specific capacitance of 1816.27 F/g at 1 A/g. The pseudocapacitive behavior of NSCF nanoparticles is further investigated using electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), and galvanostatic charge-discharge (GCD) measurements. The EIS analysis reveals a charge transfer resistance (R_{ct}) of 2.1 Ω , indicating efficient charge transfer at the electrode-electrolyte interface. The CV and GCD curves exhibit a pair of well-defined redox peaks and demonstrate a linear discharge profile, indicating ideal pseudocapacitive behavior. The nanoparticles synthesized using a L-alanine assisted sol-gel auto combustion method, followed by calcination at 1000°C. The structural and morphological properties of the nanoparticles are characterized using X-ray diffraction (XRD) confirms the formation of a cubic perovskite structure, scanning electron microscopy (SEM) confirms the porous structure provides pathways for electrolyte ions to access the materials surface, leading to efficient charge storage and Fourier Transform Infrared Spectroscopy (FTIR) provides vibration of oxygen ions and metal cations. The present study demonstrates the potential of this nanoparticle as a high-performance pseudocapacitive material for supercapacitor applications.

Keywords: Neodymium doped, Pseudocapacitive behavior, L-Alanine fuel, Auto combustion, porous structure, Perovskite material.

Analysis of Heat Treatment on the Mechanical Properties in EN Grade Steel Material

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Abstract

This cramming evaluated the impact of heat treatment on EN grade steel. EN grade steel is mostly used in machinery components, automotive parts, tooling, transmission components and construction sector. The main key grade of EN8 is mostly used for general purposes and EN24 is mostly used in heavy axles for specific strength and hardness requirements. This review focuses on the effect of heat treatment on the mechanical characteristics and microscopic structure of EN grade materials. The review also studied various heat treatment methods, such as annealing, stress relieving, spheroidizing and normalizing. In addition, the review study clarified the changes in hardness and microstructural changes of the particles.

Keywords: Mechanical properties; Microstructure; Grain refinement; Strain hardening; Heat treatment.

Energy-Efficient PET Upcycling and Hydrogen Co-Production at Industrial Current Densities via Cr-Regulated NiCoS

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Abstract

Electrocatalytic upcycling of polyethylene terephthalate (PET) waste coupled with hydrogen production provides has emerged as an attractive strategy for simultaneously addressing plastic pollution and sustainable energy generation. However, the development of efficient bifunctional electrocatalysts with mechanistic understanding remains a significant challenge. Herein, a Cr-regulated NiCoS nanosheet arrays was directly grown on nickel foam via a onestep chemical bath deposition strategy for integrated hydrogen evolution and PET hydrolysate electrolysis. Cr incorporation modulates the electronic structure of NiCoS, facilitating the rapid and reversible formation of catalytically active NiOOH/CoOOH species and accelerating interfacial charge transfer. Subsequently, the optimized catalyst delivers an HER overpotential of 257 mV at 100 mA/cm² and drives ethylene glycol oxidation at 1.326 V vs RHE, lowering the anodic potential by 176 mV as compared to oxygen evolution. Operando electrochemical measurements, and in-situ Raman spectroscopy collectively reveal an electrochemicalchemical (EC) mechanism, in which electrochemically generated oxyhydroxides are continuously consumed by EG and regenerated under anodic polarization. Benefiting from this dynamic redox process, the integrated electrolyzer achieves 10.6% lower energy consumption than conventional water electrolysis, while directly converting real PET hydrolysate into highpurity terephthalate, formate, and green hydrogen, demonstrating a practical strategy for sustainable plastic waste valorization.

Keywords: PET upcycling; Transition-metal sulphides; Electronic structure regulation; Hydrogen production; Operando spectroscopy

Self-Supported Reconstructed NiCoOx as a Bifunctional Electrocatalyst for PET Upcycling and Sustainable Hydrogen Production

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Abstract

Electrochemical upcycling of polyethylene terephthalate (PET) offers an opportunity to convert plastic-derived ethylene glycol (EG) into value-added chemicals while replacing the energy-intensive oxygen evolution reaction (OER). Herein, a self-supported NiCoOx catalyst is developed for coupling hydrogen evolution with the oxidation of PET-derived EG. The selfsupportedNiCoOx requires an HER overpotential of 210 mV at 100 mA/cm². For anodic oxidation, NiCoOx achieves 100 mA/cm² at 1.35 V vs RHE for EGOR, requiring an anodic potential 200 mV lower than that for OER. Electrochemical and in-situ Raman analyses reveal dynamic surface reconstruction, where Co/Ni-OOH serve as real active sites for oxidation of EG through an indirect-alcohol-oxidation pathway. The NiCoOx-based EG-assisted electrolyzer operates at 1.60 V, corresponding to an energy consumption of 3.90 kWh/Nm³ H₂, reducing energy consumption by 14.5% as compared to alkaline water electrolyzer. Notably, NiCoOx achieves the Faradaic efficiency of 95% for EG to formate conversion and 98% for H₂-production. The NiCoOx catalyst also maintains stable electrochemical performance at current density of 100 mA/cm² for 100 h. Overall, the NiCoOx-enabled paired electrolysis converts PET-derived EG into formate while simultaneously producing H₂ with reduced electrical energy consumption.

Keywords: Polyethylene terephthalate (PET) upcycling; Electrochemical oxidation; Ethylene glycol oxidation; Hydrogen production; Formate; NiCoOx.

OP-ESC-03

Studies On Different Air Pollutants by Using the Unmanned Aerial Vehicle (UAV) Technologies

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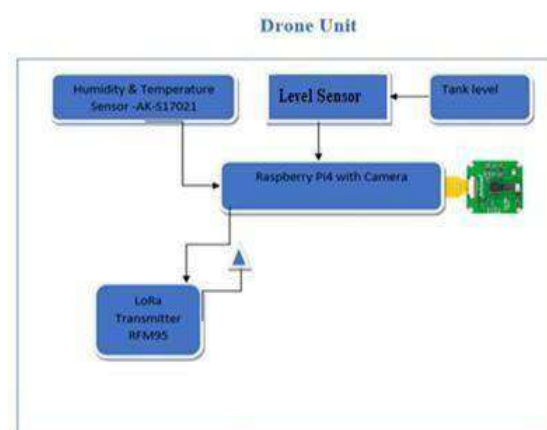
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Abstract

Atmospheric Drones are Unmanned Aerial Vehicles (UAVs) that are used to study the different air pollutants and according to a latest survey report the market for these portable drones is expected to grow at more than 44% from 2019 to 2023. The present designed UAV can be used in the study of Real Time Air Quality Monitoring, with the following features like low cost, effective solution, easy and versatile connectivity, SD card and cloud storage, reliable and accurate data, additional weather station, remote data access, hassle free set up etc., etc. The weather reports are able to get proper and actual data of the air pollutants like H₂S, NH₃, CO, NO₂, SO₂, O₃, PM₁₀, PM_{2.5} and PM₁, along with humidity and temperature values with help of different sensors embedded in atmospheric study drone. Internet of things Technology is mainly application to design artificial intelligence UAVs with low cost and low power consumption. In the present investigation we have designed a low power, low cost IOT network, explore the capability of a cost effective. Unmanned Aerial Vehicles (UAVs) for monitoring the above said environmental parameters and air pollutants. The results were compared, tabulated and conclusions were drawn.

Key Words: Atmospheric air pollutants, humidity, temperature and Unmanned Aerial Vehicles (UAVs)



OP-ESC-04

Recent Advances, Challenges and Future Perspectives on the Applications of Nanomaterials in Water Purification – A Review

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Abstract

Water pollution caused by dyes, heavy metals, pharmaceuticals, pesticides, microorganisms, and other emerging contaminants has become an important environmental problem. Conventional water-treatment methods are useful, but they may have limitations when pollutants are present at low concentrations or are difficult to degrade. Nanomaterials have received increasing attention because their small size, large surface area, tunable surface chemistry, and high reactivity can improve pollutant removal. This review summarizes important developments in the application of nanomaterials for water purification during 2020–2026, with particular attention to experimental research. Nanomaterials such as graphene oxide (GO), carbon nanotubes, metal and metal-oxide nanoparticles, nanocellulose, metal-organic frameworks (MOFs), and nanocomposite membranes have been investigated for adsorption, membrane filtration, photocatalytic degradation, disinfection, and removal of heavy metals and emerging contaminants. Reported studies show that surface-modified GO materials can achieve high dye removal, TiO₂ nanoparticles can provide photocatalytic degradation and microbial inactivation, and MOF membranes can provide highly selective separation of dyes and salts. Recent work has also moved toward sustainable nanocellulose materials and larger-scale membrane fabrication. However, practical application is still limited by material cost, nanoparticle recovery, membrane fouling, long-term stability, possible environmental toxicity, and difficulties in scaling laboratory results to real wastewater. Future research should therefore focus on stable, reusable, low-cost, and environmentally safer nanomaterials tested under realistic water-treatment conditions.

Keywords: Nanomaterials, Water Purification, Wastewater Treatment, Nano-adsorbents, Nanomembranes, Photocatalysis, Graphene Oxide, Metal Nanoparticles, Nanocellulose, Metal–Organic Frameworks.

OP-ESC-05

Histidine-Modified Poly N-Methyl aniline for Sustainable Corrosion Mitigation of Mild Steel in Acidic Environment

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Abstract

Poly aniline is an attractive material for corrosion inhibition studies. In this study, poly N-methyl aniline doped with Histidine and explored for their inhibitive action of mild steel corrosion in 0.5M Sulphuric acid. The doped polymer was evaluated using weight loss method, polarization studies and electrochemical impedance studies. The doped polymer exhibited maximum efficiency of 91.21% at the concentration 230 ppm. The inhibitor efficiency of doped increased at 3 hours of immersion followed by a decrease, and an increase at 24 hours of immersion. Potentiodynamic polarization studies indicate the polymer as mixed inhibitors. The impedance measurements and polarization studies were comparable with the weight loss studies. The synergistic action of poly aniline and doped polymer was confirmed by the synergistic parameter calculation. The changes occurred in the electrolytic solution after the immersion of mild steel samples for 6 h of immersion period was determined by Atomic absorption spectroscopy and UV-visible spectroscopic studies. The results provide some preliminary information about the complex formation in the solution phase and also the protective layer formation on the metal surface. The protective layer is characterized using Scanning electron microscopy and EDAX analysis.

Keywords: Poly aniline, Doped polymer, Histidine, mild steel, SEM

**A Critical Assessment of Green Chemistry Strategies for Transitioning
Towards a Circular and Climate Sustainable Plastics Economy**

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Abstract

The plastics economy has delivered significant societal and technological benefits, but its predominantly linear model of production, consumption and disposal has intensified fossil-resource dependence, greenhouse-gas emissions, plastic pollution, resource depletion and waste accumulation. Transitioning to a circular and climate-sustainable plastics economy requires a life-cycle approach extending beyond conventional waste management to encompass circular molecular design, safer chemicals, renewable feedstocks, energy-efficient synthesis, reuse, advanced recycling and sustainable end-of-life pathways. Green chemistry provides a scientifically robust framework for this transition by integrating environmental considerations into the design of chemicals, materials and processes. This study critically evaluates the potential, limitations and sustainability implications of green chemistry strategies for developing a circular and climate-sustainable plastics economy. Key areas examined include design for circularity, renewable feedstocks, low-carbon polymerisation, safer monomers and additives, catalytic synthesis, solvent minimisation, mechanical and chemical recycling, enzymatic depolymerisation, dissolution-based recycling, bio-based and biodegradable polymers, and carbon-efficient manufacturing. The study also highlights the importance of life-cycle assessment (LCA), techno-economic assessment (TEA), material-flow analysis and chemical-safety considerations in determining the actual environmental performance of emerging technologies. The analysis indicates that no single technology can independently address the plastics challenge. Chemical recycling can complement mechanical recycling for complex, contaminated or degraded waste streams, but its environmental performance depends strongly on energy sources, process efficiency, feedstock characteristics and LCA system boundaries. Likewise, bio-based and biodegradable plastics should not be presumed environmentally superior without comprehensive life-cycle evaluation. The study proposes an integrated Green Chemistry–Circular Plastics–Climate Sustainability Framework around five principles: prevent and reduce, redesign and substitute, retain material value, regenerate molecular resources, and assess whole-system sustainability. The framework connects green chemistry with circular economy strategies and SDGs 9, 12, 13, 14 and 15. The study concludes that sustainable plastics transition should prioritise prevention, reuse and circular design, supported by low-carbon, resource-efficient recycling. Future research should emphasise recyclable-by-design polymers, non-toxic additives, low-energy catalytic depolymerisation, renewable carbon, digital material tracking, harmonised LCA methodologies and integrated policy mechanisms. Green chemistry can thus provide the foundation for transforming the plastics life cycle towards resource efficiency, circularity and climate resilience.

OP-ESC-07

A Facile One-Pot Synthesis of imidazole compounds using Microwave Irradiation in Bisulphate-Silicate Heterogeneous Catalyst in dry media

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Abstract

An eco-friendly procedure was adopted to obtain imidazoline benzamide derivatives I-1 to I-5 from Imidazole and aromatic amide and substituted benzaldehyde in the presence of 1 equiv. of Bisulphate silicate catalyst. Conventional heating of reactants afforded the product in 62% yield in 6 h whereas microwave irradiation results the product in 74% within 3 minutes. Imidazole was found to be the most suitable compound for this synthetic transformation and Bisulphate silicate, is the ecofriendly catalyst, was used in optimal quantity for better result. Synthesized compounds are carried for IR, NMR, Elemental analysis, Insilco docking and ADME predictions. In Molecular docking studies all the compounds showed better binding score values. Synthesized compounds were screened for their antimicrobial activity and antioxidant activity. These newly synthesized compounds were evaluated by their spectral analysis.

Keywords: Imidazole, Molecular docking, ADME predictions, Antioxidant studies, Solvent-free reactions

OP-ESC-08

Physicochemical, Tensile and Thermal Characterization of New Natural Cellulosic Fibers from the Leaf of *Bacopa Monnieri*

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Abstract

Natural fibers are the one worthy substitute for replacing synthetic fibers and used as a polymer reinforcement due to their eco-friendly nature. This investigation deals with the newly identified *Bacopa monnieri* fibers (BMFs) characterized by chemical analysis, single fiber tensile test, thermogravimetric analysis (TGA/DTG), Fourier transform-infrared spectroscopy (FT-IR) analysis, X-ray diffraction (XRD), and atomic force microscopy (AFM). The chemical constituents of BMFs contain cellulose (62.52%), hemicellulose (14.63%), and lignin (17.02. %). The BMFs are thermally stable up to a temperature of 338.2°C evidenced by TGA analysis. The X-ray diffraction confirmed that BMFs were rich in cellulose fraction with a crystallinity index of 56.92%.

Keywords: Chemical analysis, Fourier transform-infrared spectroscopy analysis, X-ray diffraction, Thermo gravimetric analysis, atomic force microscopy, single fiber tensile test

OP-ESC-09

Efficient Recovery of Trace Quantities of Silver from Aqueous Solutions Using a Modified Electrodeposition-Redox Replacement Process

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Abstract

Realizing the scarce availability of silver metal to for the electrical and electronic industries or its removal from wastewater because of its toxicity, the study proposes an improved electrodeposition-redox replacement process (EDRR) for the recovery of minor quantities of silver from aqueous solutions. A packed-bed, column reactor, comprising platinum-coated alumina catalyst (Pt/Al₂O₃) is operated with hydrogen gas (H₂), nitrogen gas (N₂), and air for electrodeposition of copper, redox-replacement of silver, and oxidation of both the metals, respectively. The EDRR process is thermodynamically possible due to the large difference in the reduction potentials of copper and silver, whereas the electrodeposition of copper and oxidation of copper and silver are driven by positive and high reduction potentials of metals within a wide window of pH. A proof-of-concept with a few critical process challenges are investigated. The results obtained command on the ease of operation, costeffectiveness, and flexibility of proposed EDRR process for real-life implementation.

Keywords: Electrodeposition-redox replacement, silver recovery, Hydrometallurgy, Metal recycling, wastewater treatment.

Synthesis, Functionalization and Characterization of Polymer Nanocomposite Nanohybrids for Environmental Catalysis and Sensing Applications

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Abstract

The development of multifunctional polymer nanocomposite nanohybrids has emerged as a promising approach for addressing critical environmental challenges through advanced catalytic and sensing technologies. This proposed study focuses on the synthesis, functionalization, and characterization of polymer-based nanocomposite nanohybrids with enhanced surface, structural, optical, and electrochemical properties for environmental applications. Suitable polymer matrices such as polyethersulfone (PES), polysulfone (PSF), or polyvinylidene fluoride (PVDF) will be incorporated with selected nanofillers, including graphene oxide (GO), titanium dioxide (TiO₂), zinc oxide (ZnO), silica (SiO₂), carbon nanotubes (CNTs), and selected metal/metal oxide nanoparticles. The prepared nanohybrids will be functionalized through appropriate surface modification strategies to improve their dispersion, interfacial interaction, stability, catalytic activity, and sensing performance. Comprehensive characterization will be carried out using techniques such as Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM/FESEM), Energy Dispersive X-ray Spectroscopy (EDX), Atomic Force Microscopy (AFM), Thermogravimetric Analysis (TGA), and UV–Visible spectroscopy. The catalytic performance of the developed nanohybrids will be investigated for the degradation of selected organic pollutants and emerging contaminants in aqueous systems. In parallel, their sensing capability toward selected environmentally significant analytes, particularly toxic heavy metal ions, will be evaluated based on sensitivity, selectivity, response time, and detection limit. The synergistic interaction between the polymer matrix and nanofillers is expected to enhance both catalytic efficiency and sensing performance. The study aims to develop stable, reusable, and environmentally relevant multifunctional nanomaterials that can contribute to sustainable environmental monitoring and remediation.

Keywords: Polymer nanocomposites; Nanohybrids; Functionalization; Environmental catalysis; Chemical sensing; Heavy metal detection; Photocatalytic degradation; Graphene oxide; Metal oxide nanoparticles; Environmental remediation.

Treatment of Textile Wastewater Using Ferric Chloride (FeCl_3) Chemical Coagulation: Evaluation of Colour Removal and Process Performance

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Abstract

Textile wastewater is characterized by intense coloration and the presence of suspended solids, colloidal particles, organic matter, dyes, and other chemical constituents that can adversely affect receiving water bodies. In the present study, chemical coagulation using ferric chloride (FeCl_3) was investigated as a physicochemical treatment method for the removal of color from textile wastewater. The coagulation process was evaluated by varying relevant operational conditions, particularly coagulant dosage and pH, followed by rapid mixing, slow mixing, and sedimentation. The treatment efficiency was assessed by comparing the color of the wastewater before and after coagulation. Ferric chloride effectively destabilized the colloidal and dye-containing particles through charge neutralization and subsequent floc formation. Under the investigated treatment conditions, a maximum color removal efficiency of 92% was achieved using FeCl_3 compared to other materials, demonstrating the effectiveness of ferric chloride coagulation for decolorization of textile wastewater. The substantial reduction in color indicates that FeCl_3 can serve as an effective primary treatment or pretreatment step prior to biological, electrochemical, membrane, or other advanced treatment processes. The study demonstrates the potential of chemical coagulation for reducing the visual and dye-related pollution load of textile effluent and provides a basis for further optimization of coagulant dosage, pH, settling time, sludge production, and treatment cost.

Keywords: Textile wastewater; Ferric chloride; FeCl_3 ; Chemical coagulation; Color removal; Decolorization; Flocculation; Coagulation; Wastewater treatment; Physicochemical treatment.

OP-ESC-12

Synthesis of a Flower-Like Ag Decorated MnO₂ Nanocomposite for Efficient Photocatalysis

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Abstract

Rapid industrialization and urbanization have led to increasing water pollution, creating an urgent need for efficient and sustainable wastewater treatment technologies. In this study, flower-like manganese dioxide (MnO₂) nanocomposites were synthesized through a simple water-bath method and investigated as photocatalysts for the degradation of organic pollutants under natural solar irradiation. To enhance the photocatalytic activity of MnO₂, silver nanoparticles (Ag NPs) were deposited onto its surface, forming a MnO₂/Ag nanocomposite. The photocatalytic degradation mechanism was systematically investigated using various reactive-species scavengers and an additional oxygen source, confirming the involvement of reactive oxygen species in the degradation process. Photocatalytic experiments revealed that the MnO₂/Ag nanocomposite exhibited significantly enhanced degradation efficiency compared with pristine MnO₂. The improved photocatalytic performance is attributed to the effective trapping of photogenerated charge carriers by Ag nanoparticles, which facilitates charge separation, suppresses electron–hole recombination, and promotes the generation of reactive oxygen species. The results demonstrate that Ag loading is an effective strategy for improving the solar-light-driven photocatalytic activity of MnO₂ nanoflowers. Owing to its facile synthesis, enhanced photocatalytic efficiency, and utilization of renewable solar energy, the MnO₂/Ag nanocomposite shows considerable potential as an environmentally friendly photocatalyst for sustainable wastewater treatment.

Keywords: Nanocomposite, Photocatalysis, Reactive oxygen species, Wastewater treatment

OP-ESC-13

Green Synthesis, Characterization and Antibacterial Evaluation of Silver Nanoparticles Using *Solena amplexicaulis* Leaf Extract

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Abstract

Methanolic leaf extract of *Solena amplexicaulis* was used in an environmentally friendly method to create silver nanoparticles (AgNPs). The extract-to-silver nitrate ratio, temperature, and reaction time were varied to create three batches. AgNP formation was verified by UV-visible spectroscopy and color change. Characterization techniques included FTIR, SEM, and particle-size analyzes. For Batches A, B, and C, absorption maxima were noted at 435, 425, and 410 nm, respectively. Batch C's particles were mostly round or oval in shape, with an average size of 98.1 nm. It demonstrated inhibitory zones of 23, 8, and 31 mm against *S. aureus*, *P. aeruginosa*, and *E. coli*, respectively.

Keywords: Silver nanoparticles; green synthesis; *Solena amplexicaulis*; phytochemicals; characterization; antibacterial activity

Advanced Polymer Nanocomposite Membranes for Efficient and Sustainable Wastewater Treatment

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Abstract

The increasing generation of industrial and domestic wastewater containing heavy metals, dyes, organic pollutants, and other emerging contaminants poses significant challenges to environmental sustainability and water security. Conventional wastewater treatment methods often suffer from limitations such as high energy consumption, inadequate removal efficiency, secondary pollution, and membrane fouling. In this context, advanced polymer nanocomposite membranes have emerged as promising materials for efficient and sustainable wastewater treatment. The present study focuses on the development and characterization of polymer nanocomposite membranes by incorporating functional nanomaterials into suitable polymer matrices to improve membrane performance and contaminant removal. Polymeric membranes based on materials such as polyethersulfone (PES), polysulfone (PSF), or polyvinylidene fluoride (PVDF) will be modified with selected nanofillers, including graphene oxide (GO), titanium dioxide (TiO₂), zinc oxide (ZnO), and other functional nanomaterials. The membranes will be fabricated using an appropriate phase-inversion and/or surface-modification technique. Their structural, morphological, surface, and physicochemical properties will be investigated using FTIR, SEM/FESEM, EDX, AFM, contact-angle measurements, porosity, and mechanical-property analysis. Membrane performance will be evaluated through pure-water flux, permeability, contaminant rejection, antifouling behaviour, and reusability studies. The incorporation of nanofillers is expected to enhance membrane hydrophilicity, surface functionality, mechanical stability, water permeability, and selective pollutant removal while reducing fouling. The developed nanocomposite membranes are anticipated to provide an effective, reusable, and environmentally sustainable platform for advanced wastewater treatment and water-reuse applications.

Keywords: Polymer nanocomposite membranes; nanofillers; graphene oxide; nanofiltration; antifouling; sustainability.

Outdoor Durability of Photochromic Yttrium Oxyhydride Thin Films for Smart-Window Applications: A Field Study in a Tropical Climate

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Abstract

Photochromic rare-earth oxyhydrides are attractive as voltage-free, self-powered coatings for passive smart-window solar control. Yet, most reported performance data come from short, chamber-based tests that cannot reproduce real outdoor stresses. We report a 14-month continuous outdoor field study (January 2025–February 2026) of yttrium oxyhydride (YHO) thin films at Madurai Kamaraj University, India, a tropical site with luminosity up to 1500 lux, surface temperatures up to 60 °C, and humidity ranging from 15–70%. Seven DC reactive-magnetron-sputtered films spanned two series: three deposition pressures (0.9–1.1 Pa, fixed 635 nm thickness) and four thicknesses (430–1895 nm, fixed 1.0 Pa). Monthly UV-Vis measurements show that deposition pressure, not thickness, is the decisive parameter for outdoor photochromic durability. Only the 0.9 Pa film (P1) sustained reversible photochromism across the full annual cycle, with efficiency ranging from 22% in the dry season to 54.9% at peak summer irradiance. Raising the pressure by just 0.1 Pa collapsed average annual efficiency by 85–90%, and even the thickest film (1895 nm) never exceeded 21% efficiency. This behaviour is attributed to pressure-dependent adatom kinetics: lower pressure yields higher adatom energy and more efficient hydrogen incorporation, producing a dense, H-rich precursor whose H[−]/O^{2−} balance survives prolonged atmospheric exposure, whereas higher pressure gives a porous, H-deficient film that over-oxidises within weeks. These results establish sputtering deposition pressure as a critical, actionable design rule for durable, tropics-rated photochromic smart-window coatings, and provide one of the most extended real-world durability records reported for this materials class.

Keywords: yttrium oxyhydride; photochromic thin films; smart windows; magnetron sputtering; outdoor durability; passive solar control

OP-ESC-16

Fluoride Exposure and Mineral–Renal Biomarkers in the Palar River Bank Belt of Tamil Nadu, India

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Abstract

Fluoride exposure through drinking water may influence calcium homeostasis and renal function, particularly in populations residing in fluoride-prone areas. This cross-sectional study evaluated fluoride exposure among healthy men aged 25–35 years from ten villages in the Palar River bank belt of the erstwhile Vellore District, Tamil Nadu, India, now comprising Vellore, Tirupattur, and Ranipet districts. Of 120 men assessed, 95 were excluded because of diabetes mellitus, chronic kidney disease, vitamin D or calcium supplementation, medications affecting mineral metabolism, other systemic disorders, or incomplete information. Twenty-five eligible participants were included. Borewell and piped drinking-water samples, venous blood, and morning spot urine were collected. Fluoride concentrations in water, serum, and urine were determined using SPADNS and ion-selective electrode methods. Serum calcium, 25-hydroxyvitamin D₂, parathyroid hormone, urea, and creatinine were measured using established biochemical methods. Descriptive, correlation, and regression analyses were performed, with significance set at $p < 0.05$. The study evaluates fluoride exposure and its relationship with mineral homeostasis and renal biomarkers in this population.

Keywords: Fluoride exposure; Palar River; Vellore District; Drinking water; Serum fluoride; Urinary fluoride; Vitamin D; Calcium homeostasis; Parathyroid hormone; Renal function.

Nano-Armoured Bio Cementation for Tropical Landslide Mitigation: A High-Penetration, Eco-Compliant Framework for Wayanad Region

Kowshika R

Abstract

Monsoon-induced landslides present a catastrophic hazard in the high-rainfall, tropical terrain of Wayanad within the Western Ghats. Traditional stabilization methods are carbon-intensive and ecologically disruptive. To address this, this study introduces a site-specific geotechnical framework leveraging Nano-Armoured Microbially Induced Carbonate Precipitation (MICP) for sustainable slope stabilization. To optimize bio cementation within Wayanad's warm climate, the system deploys the thermotolerant bacterium *Sporsarcinapasteurii*. A major bottleneck in slope grouting is the premature flushing of biological agents by torrential rain. This framework resolves the washout limitation by encapsulating bacteria within protective Mesoporous Silica Nanoparticles (MSNs), providing the necessary temporal window for uniform crystallization. To ensure deep subsurface transport, polycarboxylate ether (PCE) is introduced into the suspension. The PCE imparts steric hindrance, mitigating nanoparticle agglomeration and maintaining an ultra-low viscosity fluid profile that allows the grout to flow uniformly through heterogeneous soils to reach the critical soil-bedrock interface. Upon activation, the resulting calcium carbonate matrices securely anchor loose topsoil to the underlying bedrock, forming a resilient, water-resistant shear boundary. Crucially, the environmental hazard of byproduct ammonia leaching is eliminated by integrating natural zeolites to sequester excess ammonium (NH_4^+) ions, transforming an aquatic toxin into a slow-release nutrient for slope-stabilizing vegetation. By bridging nanotechnology with localized disaster mitigation, this holistic framework presents novel, highly scalable paradigm for sustainable infrastructure preservation.

Keywords: Landslide mitigation; Wayanad; *Sporsarcinapasteurii*; mesoporous silica nanoparticles; polycarboxylate ether; low viscosity; soil-bedrock interface; zeolites

Design of Ethylene Glycol-Capped Ag–TiO₂ Nanophotocatalysts for Environmental Remediation

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Abstract

Efficient nanostructured photocatalysts are essential for the sustainable treatment of dyecontaminated wastewater. In this study, ethylene glycol (EG)-capped silver-doped TiO₂ nanostructures were synthesized by a modified sol–gel method using 1, 2, and 3 mol% Ag relative to Ti. EG served as a capping and growth-regulating agent to control particle aggregation and surface characteristics, while Ag doping was used to tune the optical and charge-carrier properties of TiO₂. The synthesized nanomaterials were characterized using UV–Visible spectroscopy, FTIR, XRD, photoluminescence, HRTEM, SAED, EDS, and BET analyses. Ag incorporation significantly improved the optical properties, reducing the band gap from 3.25 eV for EG@TiO₂ to 2.80 eV for EG@2%Ag–TiO₂. XRD confirmed crystalline TiO₂ with rutile-dominant/mixed-phase characteristics, while HRTEM revealed nanofibrous structures with an average diameter of approximately 54 nm. The optimized EG@2%Ag–TiO₂ exhibited a surface area of 47.886 m² g^{−1} and pore diameter of 2.06 nm. Photocatalytic activity was evaluated using Reactive Yellow 15 (RY15) under visible-light irradiation. EG@2%Ag–TiO₂ achieved 99.7% decolorization within 18 min, with an apparent rate constant of 0.3267 min^{−1}, compared with 73.1% and 0.0727 min^{−1} for undoped EG@TiO₂. The enhanced activity is attributed to optimized Ag incorporation, improved interfacial charge transfer, reduced electron–hole recombination, and accessible surface sites. These findings demonstrate the potential of EG-capped Ag–TiO₂ as an efficient photocatalyst for rapid wastewater treatment.

Keywords: Ag-doped TiO₂, ethylene glycol capping, nanostructures, wastewater remediation

OP-ESC-19

A Recyclable Cs/Al₂O₃ Catalyst for Green, Efficient and Facile Synthesis of Novel Morpholino-pyridine Analogues

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Abstract

New, easy to synthesize, extremely stable and environmentally friendly catalysts, cesium loaded alumina (Cs/Al₂O₃) catalyst, have been successfully synthesized. The catalyst material was characterized by various spectroscopic analyzes such as BET, TEM, SEM, P-XRD and SEM-EDS. The nanomaterial was used as a catalyst for the synthesis of morpholino-pyridine under mild reaction conditions. This green approach possesses numerous advantages such as simple operation, low cost, eco- friendliness, simple work-up, short reaction time (less than ten minutes), low waste, safer greener solvent, easy purification and high product yields (91-98%). Interestingly, the material could be easily removed from the reaction mixture by simple filtration and reused several times without loss of its activity.

Keywords: Green synthesis, Multicomponent reaction, One-pot approach, Pyridines

**Corrosive Inhibition of Piperidin-4-one Derivative on Mild Steel Corrosion
in 1NHCl media**

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Abstract

The anti-corrosive behavior of piperidin-4-one derivatives (PFOD) on mild steel in 1N HCl media was investigated by weight loss and potentiodynamic polarization (PDP) methods. The inhibitory parameters indicated the strong adsorption of piperidin-4-one derivative on mild steel (MS) surface. The PDP studies indicated that the nature of inhibitor and its adsorption followed Langmuir adsorption isotherm. The weight loss measurement indicated the comprehensive adsorption of inhibitor. The effect of temperature on the corrosion behavior with addition of the synthesized inhibitors was studied in the thermal range of 298–308 K. Moreover, the adsorption of these compounds on the carbon steel surface follows the Langmuir adsorption isotherm model indicating that the adsorption process is chemical. The results obtained indicate that PFOD can be used as a good corrosion inhibitor for mild steel in 1N HCl solution. Furthermore, the synergy of the experimental and theoretical approaches gives an insight into the mechanism of corrosion inhibition, which is essential for the development of effective strategies to inhibit the corrosion of metals in acidic media.

Keywords: Anti-corrosive, Piperidin-4-one derivatives, Mild steel, Polarization

OP-ESC-21

Seaweed-Derived Sulfated Polysaccharide–Cellulose Nanocrystal Nanocomposite Films for Sustainable Food Packaging

Janani M

Abstract

The increasing environmental burden of petroleum-derived plastics has created a need for biodegradable and renewable alternatives for food packaging. In this study, seaweed-derived sulfated polysaccharide (SP) and cellulose nanocrystals (CNC) were utilized to develop biodegradable nanocomposite films. *Sargassum wightii* biomass was used as a sustainable source for SP and cellulose, while CNC was prepared through optimized acid hydrolysis. The CNC was incorporated into the SP matrix using glycerol as a plasticizer, and the film formulation was optimized using response surface methodology. The developed SP–CNC nanocomposite films were evaluated for their structural, morphological, thermal, mechanical and barrier properties. CNC incorporation enhanced the structural stability and functional performance of the films, including improved resistance to ethanol and oil penetration. Soil burial studies demonstrated controlled biodegradation of the nanocomposite film, highlighting its environmental potential. The film was further evaluated for food-packaging applications and demonstrated suitability for protecting selected food products during storage. Overall, the study demonstrates the potential of seaweed biomass-derived polysaccharide and nanocellulose as renewable components for developing functional and sustainable biodegradable food-packaging materials.

Keywords: Seaweed; Sulfated polysaccharide; Cellulose nanocrystals; Nanocomposite film; Biodegradable packaging; Sustainable materials

OP-ESC-22

Isolation, Screening and Consortium Development of Nitrate-Degrading Microorganisms for Groundwater Remediation

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Abstract

Freshwater resources are increasingly threatened by pollution arising from various anthropogenic activities, creating a need for effective remediation to ensure their safe and sustainable utilization. Agricultural and industrial sectors extensively utilize nitrogen containing products, particularly fertilizers and explosives, resulting in the accumulation of nitrogenous compounds in surface water and groundwater. Improper application and disposal of nitrogen-based materials have significantly contributed to nitrate and ammonia contamination of aquatic environments. Nitrate-polluted groundwater poses potential direct and indirect risks to human health. Various chemical, physical, and biological approaches have been investigated for the removal of nitrate from contaminated water and soil. However, many of these methods do not effectively convert nitrate into molecular nitrogen (N_2), which is desirable for restoring the natural nitrogen cycle. In addition, conventional treatment processes may generate secondary pollutants, including chemical sludge, brine, nitrite (NO_2^-), ammonia (NH_3), and nitrous oxide (N_2O), thereby creating additional environmental concerns and treatment challenges. Biological denitrification is considered one of the most economical, efficient, and widely applied approaches for nitrate removal from groundwater. During denitrification, microorganisms reduce nitrate or nitrite under anoxic or anaerobic conditions, ultimately producing nitrogen gases, predominantly molecular nitrogen (N_2). In the present study, nitrate-degrading microorganisms were isolated from contaminated water and soil samples. The selected microbial strains were improved and enriched using a mineral salt medium, followed by the development of a microbial consortium to enhance nitrate degradation efficiency. The influence of key process parameters, including inoculum concentration, pH, and temperature, on the denitrification performance was systematically evaluated. Following the biological treatment, coagulation and disinfection processes were carried out in batch mode to facilitate the removal of microbial biomass and suspended matter from the treated water.

**Photocatalytic Degradation of Organic Pollutants Using La₂FeCoO₆
Double Perovskite: Synthesis, Mechanism, and Performance Evaluation**

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Abstract

La₂FeCoO₆, a novel double perovskite material, has attracted considerable interest for its unique properties, including its potential as a ferromagnetic semiconductor. UV-Vis diffuse reflectance spectroscopy revealed a narrow optical band gap of 1.7 eV for the synthesized La₂FeCoO₆, indicating its strong potential for visible-light-driven photocatalysis. The photocatalytic performance of La₂FeCoO₆ was evaluated through the degradation of malachite green dye under sunlight and visible light irradiation. Under sunlight irradiation, the dye solution turned completely clear, indicating near-total degradation, while under visible light, a degradation efficiency of 97% was achieved. These results highlight the strong light-harvesting and catalytic efficiency of La₂FeCoO₆ under natural and visible-light conditions. This report presents a comprehensive investigation into the photocatalytic applications of La₂FeCoO₆ double perovskite. By examining its fundamental structural, electronic, and optical properties, exploring its efficiency in degrading malachite green dye under sunlight and visible light irradiation, reviewing relevant synthesis and characterization methods, comparing its performance with other reported photocatalysts, elucidating the proposed mechanisms underlying its photocatalytic activity, and investigating its stability and reusability, this report aims to contribute to the broader understanding of La₂FeCoO₆ as a promising material for environmental photocatalysis.

OP-ESC-24

Effects of CuO and ZnO Nanoparticles on Black Soil Properties and Agricultural Efficacy

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Abstract

This study evaluates the influence of copper oxide (CuO) and zinc oxide (ZnO) nanoparticles on the structural and thermal physical properties of black soil, along with their subsequent effects on crop yield. Black soil, characterized by high clay and organic matter content, exhibits strong reactivity toward nanoparticles, leading to key structural realignments and physical modifications. Application of both nanoparticles increased soil compaction as well as overall bulk and particle density compared to the untreated control. Soil treated with ZnO recorded the highest bulk and particle density, indicating structural densification that enhances soil strength. Both nanomaterials significantly improved water holding capacity (WHC). ZnO-treated soil achieved the highest WHC (81.72%) alongside the largest pore space (38.35%), attributed to fine particle dispersion creating accessible micropores that aid aeration and root penetration. Conversely, CuO-treated soil showed lower pore space (26.39%) due to larger agglomerates filling pore voids, yet demonstrated the highest saturated moisture content (46.73%). Energy Dispersive X-ray Spectroscopy (EDS) confirmed the successful integration of CuO and ZnO nanoparticles into the soil matrix. While CuO nanoparticles enhance water saturation and heat transfer, their tendency to agglomerate slightly reduces total pore space. Overall, ZnO nanoparticles demonstrated superior improvements in water retention, pore architecture, and structural balance. Ultimately, both nanoparticle treatments improved soil physical parameters, promoting faster seed germination and enhanced crop yields, specifically demonstrated in onion cultivation.

Keywords: Black Soil, CuO Nanoparticles, ZnO Nanoparticles, Water Holding Capacity, Bulk Density, Porosity, Thermal Conductivity, Soil Aggregation.

OP-ESC-25

Enhanced Nitrate Removal from Contaminated Water Using Microbial Consortium

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Abstract

Freshwater is a scarce resource that continues to be at high risk of pollution from anthropogenic activities, requiring remediation in such cases for its continuous use. The agricultural and industrial activities extensively use water and nitrogen dependent products, mainly in fertilizers and explosives, respectively, with their excess accumulating in different water bodies. The intensive use of nitrogen-based products and their inappropriate disposal has contributed to ammonia and nitrate contamination of both surface and groundwater source. Ground water contaminated by nitrate will cause direct or indirect harm to human health. Although removal of nitrate from water and soil through the application of chemical, physical, and biological methods has been studied globally, these methods seldom yield N_2 gas as a desired by product for nitrogen cycling. These methods predominantly cause secondary contamination with deposits of chemical waste such as slurry brine, nitrite (NO_2), ammonia (NH_3), and nitrous oxide (N_2O), which are also harmful and fastidious to remove. Biological denitrification is currently the most economical, effective and widely used ground water nitrate removal technology. In this process Nitrate or nitrite nitrogen being reduced by microorganisms to nitrogen oxides or nitrogen (N_2) under anoxic or anaerobic conditions. In this study nitrate degrading organisms were collected from the contaminated water and soil sample. Improvement of microbial strain was done by using mineral salt medium and microbial consortium was developed to enhance the degradation of nitrate. Effects of various parameters such as inoculum concentration, pH and temperature on denitrification process were also studied. Coagulation and disinfectant process for removal of microorganisms and suspended matter were carried out in batch mode process.

OP-ESC-26

**Bismuth oxybromide-green synthesized ZnO 3d microsphere
Nanocomposite for Degradation of Carbamazepine**

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Abstract

Carbamazepine (CBZ) is a persistent pharmaceutical pollutant requiring sustainable degradation strategies. This study develops a novel photocatalyst by integrating Bismuth oxybromide (BiOBr) with green-synthesized Zinc Oxide (ZnO) 3D microspheres. The ZnO microspheres were prepared using an eco-friendly plant extract approach, followed by the fabrication of the BiOBr/ZnO heterojunction via a facile precipitation method. Characterization confirmed the uniform decoration of BiOBr on the ZnO hierarchical structure. Photocatalytic evaluations demonstrated that the BiOBr/ZnO nanocomposite exhibited significantly enhanced visible-light degradation of CBZ compared to pristine ZnO and BiOBr. This improvement is attributed to expanded visible-light absorption and efficient separation of photo-induced electron-hole pairs. The highly stable and reusable nanocomposite presents an environmentally benign and promising solution for pharmaceutical wastewater remediation.

Keywords: Bismuth oxybromide, Green synthesis, ZnO 3D microspheres, Carbamazepine

OP-ESC-27

Integrated Application of Seaweed-Derived Calcium Carbonate and Ca-Doped ZnO for Sodic Soil Reclamation and Plant Growth Enhancement

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Abstract

Sodic soils are a significant constraint to agricultural productivity owing to excessive sodium accumulation, soil structural deterioration, nutrient imbalance, and impaired plant growth. The present study investigated a sustainable approach for sodic soil reclamation using calcium-rich materials derived from the marine macroalga *Halimeda macroloba* in combination with calcium-doped zinc oxide (Ca-doped ZnO) nanoparticles. Calcium carbonate (CaCO₃) obtained from *H. macroloba* was converted to calcium oxide (CaO) through calcination, while Ca-doped ZnO nanoparticles were synthesized and characterized using UV–Visible spectroscopy, FTIR, EDX, SEM, XRD, and TGA analyses. The synthesized materials were subsequently applied to sodic soil to assess their effects on soil physicochemical properties and the early growth of green gram (*Vigna radiata*). Soil pH, electrical conductivity (EC), exchangeable sodium percentage (ESP), and nutrient characteristics were evaluated before and after treatment. The ESP declined from 14.57 on day 1 to 7.03 on day 20, indicating a substantial reduction in soil sodicity. Similarly, soil pH decreased from 9.8 to 7.5, while EC declined from 7.6 to 2.3 mS cm⁻¹ following treatment. Groundnut showed progressive establishment throughout the 20-day evaluation period, attaining approximately 11 cm in height with well-developed leaves by day 20. Overall, the findings highlight the potential of *H. macroloba*-derived calcium materials coupled with Ca-doped ZnO nanoparticles as an eco-friendly and sustainable strategy for improving sodic soil conditions and supporting crop establishment.

Keywords: *Halimeda macroloba*; Ca-doped ZnO nanoparticles; Sodic soil reclamation; *Vigna radiata*; Sustainable agriculture.

Fabrication of Nano Silver Oxide–Moringa Gum–Lavender Oil Nanocomposite Biofilms for Antimicrobial Food Packaging

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Abstract

Nano silver oxide (0.5g) was blend with moringa gum - lavender oil to get a homogenous nanocomposite film by solution cast method. Three different biofilms were synthesised (Pristine moringa gum film, nano silver oxide + moringa gum film and lavender oil + nano silver oxide + moringa gum film) and comparative studies were done. The morphology of the biofilms was studied using scanning electron microscope (SEM). Physio-mechanical properties were analysed and compared with the pristine film. From the obtained results, it was found that the water solubility, thickness, transparency, mechanical strength, antibacterial activity of the prepared composite films showed better improvement when compared to the parent film. On exact comparison, lavender oil + nano silver oxide + moringa gum composite film gave overall best result that was followed by nano silver oxide + moringa gum composite film and pure moringa gum film due to the interaction of their functional groups. Thus, the synthesised films hope to act as an ideal material for food packaging application.

Keywords: Nano Silver Oxide, Moringa Gum, Lavender oil, Biofilm, Food packaging

OP-ESC-29

Au Nanoparticles-coated TiO₂ Nanotubes for Boosting Photocatalytic Degradation of Malachite Green Dye Under Sunlight

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Abstract

In this study, titanium dioxide nanotube arrays were anodized at different applied voltages to investigate the effect of the nanotube geometry on the optical absorption and photocatalytic activity. An optimum anodization voltage was determined within the range 40 V-70 V by the physical investigations of the nanotube geometry of TiO₂ nanotubes. The diameter of 40 V-70 V samples ranged between 100-173 nm. Crystallinity in the TiO₂ nanotubes was induced by annealing at 450 °C. Gold nanoparticles (AuNPs) were coated onto the surface of TiO₂ nanotubes to improve their visible light absorption and photoactivation under sunlight. The optical absorption of nanotubes changed accordingly with the diameter of the nanotubes. The influence of anodization voltage on the photocatalytic activity of the AuNPs-coated TiO₂ nanotubes was studied using the malachite green (MG) dye. The results showed that the variation in the nanotube diameter significantly impacted the optical absorption property, crystallinity, and photocatalytic activity of the AuNPs-coated TiO₂ nanotubes. Compared to nanotubes formed at 70 V, increased photocatalytic activity was observed in the nanotubes prepared at 40 V due to better optical absorption from specific nanotube geometry and surface morphology.

Keywords: Titanium dioxide nanotubes, photocatalysis, malachite green, gold nanoparticles, sunlight.

A Study on Students' Behaviour Towards Not Attending College

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Abstract

Student absenteeism is a persistent concern in higher education because irregular attendance can influence academic engagement, classroom interaction and students' overall learning experience. This paper examines the possible factors associated with students' decisions not to attend college regularly. The study considers academic motivation, teaching-learning practices, peer influence, commuting difficulties, personal responsibilities, digital learning preferences and perceptions of attendance requirements. A descriptive research framework is proposed, supported by an illustrative questionnaire-based dataset of 120 students. The illustrative analysis indicates that lack of perceived relevance of classes, preference for online learning resources, transport-related difficulties, peer influence and personal commitments may contribute to non-attendance. The paper argues that absenteeism should be approached as a multidimensional behavioural and institutional issue rather than solely as a disciplinary problem. The study recommends stronger mentoring, interactive pedagogy, early identification of absenteeism, student feedback mechanisms and targeted academic support. The numerical data in this paper are synthetic and are provided only to demonstrate the structure and interpretation of a journal-style study; they are not actual institutional survey results.

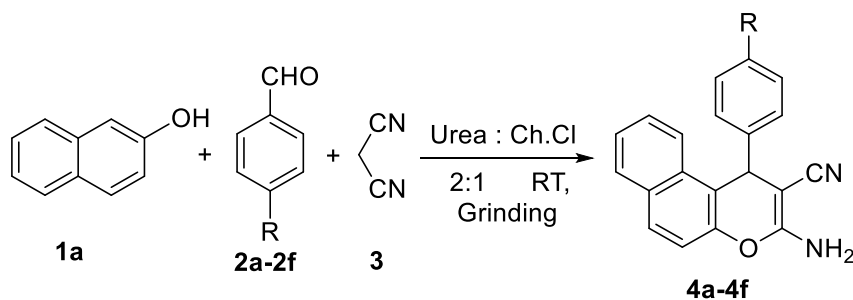
Keywords: Student absenteeism; college attendance; student behaviour; higher education; academic engagement; student motivation; teaching-learning; institutional support

A Greener Multicomponent Synthesis of Benzochromenes

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Chromenes are fused heterocyclic compound consisting of a pyran and benzene ring. Due of their biological potentials such as anticancer, anti CNS disorders, and antiviral activities, benzochromene synthesis was found to be an important task for synthetic organic chemist. Green solvents were developed as a more environmentally friendly alternative to petrochemical solvents. In connection of organic synthesis with green solvent, the present study aimed to develop a green protocol to construct the synthesis of benzochromene and spirobenzochromenes using Deep Eutectic Solvent (DES) as a green solvent at room temperature. Various organic transformations such as Knoevenagel–hetero-Diels–Alder reaction, has been catalysed by DES. Therefore, we have extended our present research work by employing DES as a green solvent, because it has tremendous advantages such as inexpensive, capable of dissolving many polar organic compounds, easier product separation and excellent yields of the product with shorter reaction time. From our work, we have evidence that DES an efficient greener solvent for various organic transformation in organic synthesis. DES is able to form strong hydrogen bond networks with various compounds might be the reason for its potentiality as a green solvent. We have synthesized benzochromene and spirobenzochromenes derivatives via multicomponent reaction in presence of DES as a solvent. The reaction was found to be proceeded in an efficient manner within a short duration of time.



OP-ESC-32

Comparative Study on Pharmacological Potential of TiO_2 Nanoparticles from Edible Plants by Chemical and Green Methods

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Abstract

In recent years, nanoparticles have materialized vital role in medicine, with various uses in clinical, drug and gene conveyance. In the present study, Two different methods (Sol-gel & biological) were adopted for synthesis of TiO_2 nanoparticles prepared from the leaf extracts of MollungoOppositifolia and TrianthemaPortulacastrum were compared with the chemical TiO_2 -nanoparicles for antibacterial and antioxidant activities. The Synthesized TiO_2 – NPs are evaluated for antimicrobial and antioxidant activities. Green TiO_2 – NPs has antibacterial effect against psedomonasaeruginosa (17+0.56 micro ml) and staphylococuss aureus (16+0.24-micro ml) at concentrations as low as 100ml. TiO_2 - NPS Prepared from green methods represents eco – friendly properties that aid in the degradation of toxic dyes due to their antionoxidant activity. Hence TiO_2 prepared through green method provides 4.5 times higher potency than chemical methods in this plants.

Keywords: Nano Particles, Mollugo Oppuositifolia, Trianthema Portulacastrum, Antioxidants, Phyto – active compounds TiO_2 - antibacteria

OP-ESC-33

Synthesis, Characterization and Computational Investigation of Cobalt (II) complex of *N,N'-(1,2-phenylene)bis(1-(5-bromothiophene-2-yl)ethane-1-imine)*

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Abstract

This work reports the synthesis, characterization, and biological evaluation of a Cobalt(II) complex with a novel Schiff base ligand, *N,N'-(1,2-phenylene)bis(1-(5-bromothiophene-2-yl)ethane-1-imine)* (PBTE). The ligand was synthesized by condensation of *o*-phenylenediamine with 2-acetyl-5-bromothiophene, followed by the formation of its Co(II) complex in a 1:1 molar ratio. The structures of the ligand and complex were characterized using FT-IR, UV-Vis, ¹H-NMR spectroscopy, elemental analysis, molar conductance and magnetic moment measurements. Spectral studies indicated coordination through azomethine nitrogen and thiophene sulfur atoms, suggesting a distorted octahedral geometry for the Co(II) complex. Computational studies using the PM6 semi-empirical method provided optimized geometries and electronic properties, showing good agreement with experimental results. The complex exhibited enhanced non-linear optical (NLO) properties compared to the free ligand. Biological studies revealed that the Co(II) complex shows improved antibacterial and antioxidant (DPPH radical scavenging) activities relative to the ligand. These findings demonstrate that metal coordination significantly enhances the biological and optical properties of Schiff base derivatives.

Keywords: Schiff base, Cobalt(II) complex, PBTE, PM6 method, NLO properties, Antibacterial activity, Antioxidant activity.

OP-ESC-34

Synthesis of Copper Oxide and Zinc Oxide Nanoparticles Using *Cardiospermum Halicacabum* leaf Extract

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Abstract

The present study focuses on the green synthesis, characterization and antibacterial evaluation of copper oxide (CuO) and zinc oxide (ZnO) nanoparticles using *Cardiospermum halicacabum* leaf extract as a natural reducing and stabilizing agent. The use of plant-mediated synthesis provides an eco-friendly and cost-effective alternative to conventional nanoparticle synthesis methods involving hazardous chemicals. Fresh leaves of *Cardiospermum halicacabum* were used for the preparation of an aqueous leaf extract. CuO and ZnO nanoparticles were synthesized using copper nitrate trihydrate and zinc nitrate hexahydrate, respectively, followed by alkaline precipitation using sodium hydroxide. The synthesized nanoparticles were characterized using Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDX) and Fourier Transform Infrared Spectroscopy (FTIR) to investigate their morphology, elemental composition and functional groups. SEM analysis revealed aggregated and irregular morphologies, including flake-like and plate-like structures, for the synthesized CuO and ZnO nanoparticles. EDX analysis confirmed the presence of copper and oxygen in CuO nanoparticles and zinc and oxygen in ZnO nanoparticles, with carbon and other minor elements attributed to phytochemical residues from the plant extract. The antibacterial activity of the synthesized nanoparticles was evaluated by the well diffusion method against *Escherichia coli*, *Staphylococcus aureus* and *Klebsiella* sp. at different concentrations, using streptomycin as the positive control. The study demonstrates the potential of *Cardiospermum halicacabum* leaf extract as a sustainable biological resource for the synthesis of metal oxide nanoparticles with potential antibacterial applications.

Polymer -Based Nanocomposites for Advanced Water Purification

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Abstract

Water pollution caused by heavy metals, organic dyes, and emerging contaminants is a major environmental concern. Conventional water treatment techniques have limitations such as high cost, lower efficiency, and the generation of secondary pollutants. In recent years, polymerbased nanocomposites have gained significant attention as effective materials for advanced water purification. This review highlights recent developments from 2021 to 2026 in the field of polymer-based nanocomposites for water purification. Recent studies have investigated the synthesis of biopolymer-based nanocomposites, particularly cellulose acetate incorporated with TiO₂ nanoparticles. The prepared nanocomposites have been characterized using SEM, HRTEM, XRD, EDX, and BET analysis. The incorporation of nanoparticles into cellulose acetate can improve the surface area, adsorption capacity, photocatalytic activity, and stability of the polymer matrix. These nanocomposites have demonstrated potential for the removal of heavy metals such as lead and chromium and the degradation of organic dyes such as methylene blue (MB) and rhodamine B (RB) from contaminated water. This review also discusses the mechanisms of pollutant removal, advantages, limitations, and future prospects of polymer-based nanocomposites for sustainable water purification. Overall, polymer-based nanocomposites offer a promising approach for the development of efficient and environmentally friendly water treatment technologies.

Keywords: Eco-friendly, polymer-based nanocomposites, cellulose acetate, TiO₂ nanoparticles, photocatalytic activity, heavy metals, organic dyes, water purification.

Green Synthesis and Characterization of Silver Nanoparticles of

Phyllanthus Maderspatensis Linn

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Abstract

Breast cancer is the second leading cause of death in women around worldwide. Nanotechnology is more effective method for herbal drug delivery to the tumor tissues. In this present study an attempt was made to synthesis silver nanoparticle from *Phyllanthus Maderspatensis Linn*. It is known as madras leaf flower hence it also called as mela nelli, in tamil, which belongs to the family Phyllanthaceae has largest genus Phyllanthus. This plant was reported to have wound healing property, anti inflammatory, antimicrobial and anticancer activity and traditionally used for treating headache, brochitis, earache, and ophthalmia. The phytochemical analysis of plant extract, revealed the presence of alkaloids, flavonoids, terpenoids, phenols, tannins, glycosides, steroid, saponins and carbohydrates. The silver nanoparticles of the plant extract were prepared and characterized by UV- visible spectroscopy, FTIR analysis SEM and HR-TEM. The synthesised silver nanoparticles were evaluated for its *in-vitro* cytotoxic studies by using MCF-7 cancer cell line. The formation of Silver nanoparticles were confirmed by using UV-visible spectroscopy, FTIR analysis, SEM analysis. The spherical shape of silver nanoparticles of size in the range of 100-200 nm, confirmed by SEM and TEM analysis. The *in-vitro* cytotoxicity studies of the synthesised nanoparticles showed 88 % cell viability against breast cancer cell lines using MTT assay. The study highlights the effect of synthesised silver nanoparticles of *Phyllanthus Maderspatensis Linn* against the MCF-7 cell lines. From the study it was concluded that the potential chemoprotective activity of synthesised silver nanoparticles of *Phyllanthus Maderspatensis Linn* in a rapid and eco-friendly approach.

Keywords: *Phyllanthus Maderspatensis Linn*, Breast cancer, Silver nanoparticles, *In vitro*-cytotoxicity studies, MCF-7 cell line.

Cu(II) Complex of Glycinate-Appended Dipicolylamine as Promising Functional Mimic for Phenoxazinone Synthase

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Abstract

Copper-containing metalloenzymes play important roles in biologically relevant oxidation processes, in which copper centres facilitate electron transfer and oxygen-dependent substrate transformations. Inspired by the catalytic function of phenoxazinone synthase (PHS), in this work, we design and synthesis of Cu(II) complexes of the type [Cu(L1-2)(H₂O)](ClO₄)₂ (C1&C2), where L1&L2 are ethyl bis(pyridine-2-ylmethyl)glycinate and bis(pyridine-2ylmethyl)amine and investigated as functional biomimetic models for PHS. The complexes were characterised by HR-MS, FT-IR, UV–visible spectroscopy, and cyclic voltammetry. C1 and C2 exhibited Cu-centred redox potentials, with $E_{1/2}$ values of -0.029 and -0.508 V, respectively. The distinct electrochemical responses of C1 and C2 upon *o*-aminophenol (OAP) addition suggest that the coordination environment of the Cu centre changes when the substrate interacts with Cu. In the present context, our main aim is to examine the importance of the carbonyl group in the enzymatic oxidation of OAP to phenoxazinone and compare it with that of the C2 without a substituent at the NH position. Both complexes exhibited catalytic activity, and the reaction kinetics were evaluated using the Michaelis–Menten equation. Interestingly, C1 exhibited a V_{max} of $1.85 \times 10^{-3} \text{ M s}^{-1}$, K_m of 0.32 M, k_{cat} of 66600 h^{-1} and k_{cat}/K_m of 56.77, whereas C2 showed a V_{max} of $2.76 \times 10^{-3} \text{ M s}^{-1}$, K_m of 0.91 M, k_{cat} of 99360 h^{-1} and k_{cat}/K_m of 30.27. The substrate scope was further explored using 2-amino-4-methylphenol, which underwent catalytic oxidation to the corresponding substituted phenoxazinone product. Interestingly, glycinate-appended, C1, exhibits higher catalytic efficiency than C2; it clearly highlights the potential of these complexes as functional biomimetic models for PHS-like oxidative catalysis.

Keywords: Phenoxazinone synthase, Cu(II) complex, Biomimetic catalysis

**Green Seaweed-Mediated Synthesis of Bimetallic Nanoparticles:
Characterization and Biological potential of *Gracilaria edulis***

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Abstract

Gracilaria edulis which belongs to the family Gracilariaceae is a seaweed that grows along the southeast coast of India. It is a nutrient-rich seaweed containing various bioactive compounds with potential antimicrobial properties. In this study an aqueous extract from *G. Edulis* was employed to produce bimetallic copper–zinc (Cu–Zn) nanoparticles by a synthesis method. The plant compounds present in the extract acted as both reducing agents and stabilizing agents during the formation of the Cu–Zn nanoparticles. The resulting Cu–Zn nanoparticles were examined with techniques. UV–visible spectroscopy was employed to confirm the formation of the Cu–Zn nanoparticles by detecting absorption peaks and surface plasmon resonance bands. Fourier-transform infrared (FTIR) spectroscopy helped identify the groups involved in the formation and stabilization of the Cu–Zn nanoparticles. Scanning electron microscopy (SEM) was used to observe the shape and surface features of the Cu–Zn nanoparticles. X-ray diffraction (XRD) analysis revealed the crystalline structure of the Cu–Zn nanoparticles. To test the effectiveness of both the *G. edulis* extract and the Cu–Zn nanoparticles an evaluation was conducted using the agar-well diffusion method. The results showed that the algal extract possessed activity but the bimetallic Cu–Zn nanoparticles proved to be more effective. The Cu–Zn nanoparticles outperformed the copper nanoparticles and zinc nanoparticles in killing bacteria. This finding suggests that combining copper and zinc enhances the performance of the Cu–Zn nanoparticles.

Keywords: Green synthesis, Seaweed extract, Biometallic nanoparticles, Antimicrobial activity.

OP-ESC-39

Extracellular bio-synthesis of silver-nanoparticles by the use of shape directing surfactant

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Abstract

The effect of cetyltrimethylammonium bromide, CTAB has been studied on the optical properties and morphology of extracellular bio-synthesis of silver-nanoparticles (AgNPs) using fresh green *Oriental plane* leaves extract as a reducing, capping and stabilizing agent. The formation of Ag-nanodisks like structures was observed and/or monitored by measuring the UV-vis. spectra at different time intervals after adding the leaves extract to the different AgNO₃ solutions. In the presence of CTAB, the peak at 453 nm is shifted to shorter wavelength, i.e., 428 nm and sharpness of the surface resonance plasmon (SRP) band also decreases with time. By the use of surfactant results also confirm a significant change in the morphology and/or agglomeration tendency of AgNPs. Transmission electron microscopy (TEM) results show the formation of stable AgNPs at different concentration of AgNO₃ gives mostly spherical and/or disk like particles with diameter ranging from 12 to 35 nm.

Keywords: *CTAB, Oriental plane; Silver particles; Morphology; Kinetics*

OP-ESC-40

Isolation and Spectral Analysis of Alkaloids Present in the Ethanolic Extract of Leaves of *Rhinacanthus Nasutus*

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Abstract

Phytochemicals in plants are present in the form of isoprenoid derivatives (terpenes, terpenoids, tocopherols, tocotrienols, saponins, carotenoids) phenol compounds (lignins, coumarins, anthrocynins, tannins, isoflavones, flavonones, gingerol, flavonoids), carbohydrate derivatives (nonstarch polysaccharides, oligosaccharides, vitamin C), fatty acids (MUFA, PUFA, sphingolipids, lecithins) amino acid derivatives (pectin, capsaicnoids, genestein, epigallates, lycopene allyl-S-compounds, isothiocyanates, choline, indols) etc. The alkaloid present in the leaves of *Rhinacanthus nasutus* are isolated and studied by using spectral techniques. The plant material is sourced along the banks of Thamirabharani River near Kuzhithurai. The main objective of the present study is to isolate the active component in the leaves of *Rhinacanthus nasutus* and structural characterization of the alkaloid extracted using various spectral study techniques like Ultraviolet Spectroscopy, Infra-Red Spectroscopy, Nuclear Magnetic Resonance Spectroscopy, Mass Spectrometry

Keywords: Phytochemicals, *Rhinacanthus nasutus*, alkaloid, Ultraviolet Spectroscopy, Infra-Red Spectroscopy, Nuclear Magnetic Resonance Spectroscopy, Mass Spectrometry

OP-ESC-41

Design, Synthesis, Characterization and Computational Evaluation of Functionalized Biphenyl Derivatives via Coupling Reactions

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Abstract

The present research focuses on the design, synthesis, characterization and computational evaluation of functionalized biphenyl derivatives via coupling reactions. Suzuki–Miyaura coupling was employed as a key strategy for constructing carbon–carbon bonds using selected aryl halides and boronic acid ester in the presence of palladium catalysts. The resulting biphenyl intermediates were further treated with different carboxylic acids to introduce a series of novel functionalized biphenyl derivatives via acid-amine coupling. The synthesized compounds were purified and characterized using FT-IR, UV, ¹H NMR, ¹³C NMR and LC-MS techniques. The structural and spectroscopic data were correlated to establish the molecular structures of the synthesized derivatives. The compounds were subsequently subjected to molecular docking studies against metabotropic glutamate receptor 5 (mGlu5) to investigate their potential binding interactions. Binding modes, hydrogen bonding, hydrophobic interactions and other relevant ligand–receptor interactions will be analyzed. Furthermore, ADMET and drug-likeness studies will be performed to assess the predicted pharmacokinetic and physicochemical properties of the synthesized molecules. The integrated experimental and computational approach will provide insights into the structure–property and structure–binding relationships of the developed compounds. The study is expected to identify promising functionalized biphenyl scaffolds for further investigation in mGlu5-targeted medicinal chemistry.

Keywords: Biphenyl derivatives, Suzuki–Miyaura coupling, Amide coupling, Molecular docking, mGlu5 receptor.

Theoretical Prediction of Thermoelastic Properties of Some Fluorite Structured Solids

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Abstract

This study presents a theoretical investigation of the thermoelastic properties of selected fluorite-structured solids using different equations of state (EOS). Fluorite-type materials are of considerable interest because of their structural stability and characteristic response to changes in temperature and pressure. In this work, the pressure dependent properties of these solids are studied within a theoretical framework, with particular emphasis on the bulk modulus, pressure derivative of the bulk modulus at different pressures. Different EOS formulations are used to describe the variation of volume with pressure to examine their ability to reproduce the thermoelastic behaviour of fluorite-structured materials. The theoretical results are compared with available experimental and reported theoretical data wherever possible. A comparison of the results obtained from different EOS models helps in identifying their applicability and limitations for describing fluorite-structured solids. The study provides useful theoretical insight into the behaviour of these materials under high-pressure conditions and may be helpful in predicting their thermoelastic properties when experimental measurements are difficult or unavailable.

Keywords: fluorite-structured solids, thermoelastic properties, equations of state, bulk modulus.

OP-ESC-43

Antioxidant Potential of Urolithin Produced by *Bifidobacterium* probiotic from Human Colostrum

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Abstract

Urolithins are bioactive microbial metabolites and one of the natural source of antioxidants, derived from ellagitannins and ellagic acid. There is an ever increasing interest in their potential therapeutic applications. The concentrated urolithin product demonstrated potential applications across various fields, including anti-aging, anticancer activity and support muscle growth, metabolic and cardiovascular health, along with industrial and probiotic applications. This study investigates the production of urolithin by *Bifidobacterium* *sp* isolated from breast milk of human volunteers and evaluates its potential role as a microbial product with biomedical significance. The isolated strains were pure cultured on MRS (DeMan, Rogosa, Sharpe) agar under anaerobic conditions with 5% CO₂ and characterized based on Microbiological lab tests i.e., hemolysis pattern on blood agar, gelatin hydrolysis, and growth at varying pH, temperature and NaCl concentration ranges. Antagonistic activity against pathogenic organisms and antibiotic susceptibility were also assessed. Pomegranate dried peel powder was used as a substrate for ellagic acid extraction under reflux conditions using a Soxhlet apparatus with ethanol, methanol, and ethyl acetate containing 10% water. The extract was purified using ethyl acetate and analyzed by HPLC at 360 nm. Isolated *Bifidobacterium* strains were inoculated into BHI broth supplemented with 20 mg/L ellagic acid and 0.05 mg/L L-cysteine and incubated under anaerobic conditions to facilitate biotransformation. The derived metabolites were obtained as cell-free extracts through sequential extraction with diethyl ether and ethyl acetate. Urolithin production was confirmed by optical density measurements and verified through HPLC analysis in the range of 210–450 nm. While performing the anti-oxidant testing using DPPH with different concentrations as 500, 300 and 100 µl resulted in 64.70%, 50.53% and 42.10% free radical reduction appropriately. A comparison of urolithin from natural Pomegranate peel expressed greater free - radicals scavenging activity than commercially available Pomegranate peel's urolithin. These findings highlight the importance of microbiome-derived metabolites as enzyme modulators in the gut for production of useful metabolites for human health. This study suggests that urolithin may serve as a promising free radicals scavenger with broad therapeutic and biotechnological relevance.

Keywords: Urolithin; microbial metabolite; free radicals; *Bifidobacterium* *species*; Ellagic acid;

OP-ESC-44

***In-Silico* Screening and Pharmacokinetic Prediction of Antioxidant-Rich Kullakar Rice Constituents Against Free Radical Generating Enzymes**

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Abstract

Oxidative stress occurs when the production of reactive oxygen species (ROS) exceeds the body's antioxidant defences. It is associated with aging, cardiovascular disease, diabetes, cancer and neurodegenerative disorders. NADPH oxidase and xanthine oxidase are two major enzymatic sources of superoxide radicals, so inhibiting them is a rational way to limit ROS generation. Kullakar rice, a traditional red rice of Tamil Nadu, is rich in phenolic and flavonoid compounds with reported antioxidant activity. This study therefore screened five phytochemicals reported from Kullakar rice against NADPH oxidase (PDB ID: 8WEJ) and xanthine oxidase (PDB ID: 1FIQ) by *in silico* molecular docking, using apocynin as the standard inhibitor. The ligands were drawn in ChemDraw, energy-minimized with the MMFF94 force field and converted to PDB format with Open Babel. Docking is performed using 10 runs of the Lamarckian genetic algorithms with the grid box sized 40x40x40 and 0.375 Å spacing on Autodock software 1.5.6. The results of docking are then analysed using Autodock tools software, Bio-Via discovery studio and the interaction is also visualized using Molegro molecular viewer. All compounds bound within the active sites of both enzymes through hydrogen bonding, hydrophobic and van der Waals interactions. Among them, stigmaterol was the best compound, showing the strongest binding affinity toward both NADPH oxidase and xanthine oxidase compare with the standard. It was stabilized mainly by hydrophobic alkyl, π -alkyl and π -sigma interactions within the binding pocket. Remaining compound also bound strongly with both the enzymes, this dual-target screening highlights the therapeutic promise of Kullakar rice in mitigating oxidative stress with drug-like potential. Pharmacokinetic behavior, including oral absorption and drug-likeness, was further predicted using the SwissADME webtool. The findings not only validate the traditional health benefits attributed to this rice variety but also establish a scientific foundation for its advancement as a functional food with drug-like potential, paving the way for novel antioxidant therapies against oxidative stress-related disorders.

Keywords: Kullakar rice, NADPH oxidase, xanthine oxidase, molecular docking, antioxidant, oxidative stress, SwissADME.

Thermophysical Properties of Nanomaterials: A Theoretical Review

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Abstract

Nanomaterials exhibit remarkable size-dependent thermophysical and thermodynamic properties due to their high surface-to-volume ratio, surface energy, atomic coordination, and nanoscale interactions. This review presents a theoretical analysis of the reported studies on the size and shape dependence of important thermophysical properties of nanomaterials. Particular emphasis is placed on melting temperature, Debye temperature, cohesive energy, melting entropy, specific heat capacity, and thermal conductivity. Theoretical models based on surface energy, cohesive energy, classical thermodynamics, Lindemann's criterion have been employed to explain the deviation of nanoscale properties from their bulk counterparts. The reviewed studies indicate that melting temperature and Debye temperature generally decrease with decreasing particle size, whereas specific heat capacity may increase significantly at smaller dimensions. The dependence of melting temperature on the reciprocal particle size and the influence of particle morphology and packing fraction demonstrate the importance of surface atoms in nanoscale systems. Theoretical predictions generally show reasonable agreement with available experimental and simulation results, supporting the validity of size-dependent models. Overall, the reviewed literature demonstrates that nanoscale dimensions strongly modify thermophysical behavior and provides a theoretical basis for developing predictive models for nanomaterials used in nanotechnology, energy systems, magnetic devices, electronics, sensors, and advanced nanoscale applications. Nanoparticles can be designed to deliver drugs specifically to target cells, reducing side effects and improving treatment efficacy.

Keywords: Nanomaterials, thermophysical properties, melting temperature, Debye temperature, cohesive energy.

Biomass-Derived Silica Nanoparticles from Coconut Bark Ash for Photocatalytic Environmental Remediation

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Abstract

The present study explores the sustainable valorization of coconut bark waste as a precursor for the synthesis of silica nanoparticles and their potential application in environmental remediation. Coconut bark ash was used as a silica source, and silica nanoparticles were prepared through a sol–gel method. The synthesized material was characterized using UV–Visible spectroscopy, Fourier Transform Infrared (FTIR) spectroscopy, X-ray Diffraction (XRD), and Scanning Electron Microscopy coupled with Energy Dispersive X-ray analysis (SEM–EDX). FTIR analysis indicated the presence of surface functional groups associated with silanol and siloxane species, while XRD and SEM–EDX analyses supported the formation of nanoscale silica with predominantly spherical morphology. The study also investigated the photocatalytic degradation of methylene blue under visible-light irradiation at different pH conditions. The synthesized nanosilica exhibited photocatalytic activity over the investigated pH range, with the highest methylene blue degradation of 28.54% at pH 9. The findings demonstrate that coconut bark can serve as an inexpensive and sustainable biomass-derived raw material for producing functional silica nanomaterials. The synthesized nanosilica shows potential for application in wastewater treatment and environmental remediation. Overall, the work provides a sustainable approach for converting agricultural biomass waste into a value-added nanomaterial, supporting green chemistry principles, waste valorization, and circular-economy approaches.

Key words: Coconut bark ash; Silica nanoparticles; Green synthesis; Sol–gel method; Nanomaterials; FTIR spectroscopy; Methylene blue; Environmental remediation.

Green Synthesis and Physicochemical Characterization of Silver-Based Nanomaterials Using *Halophila decipiens* Extract

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Abstract

Marine seagrasses, long overlooked as a nanomaterial feedstock, offer a green and sustainable route to synthesizing functional silver-based nanomaterials. This study investigated the synthesis and physicochemical characterization of silver-based nanomaterials using aqueous and ethanolic extracts of *Halophila decipiens*. Synthesis conditions were optimized by varying AgNO₃ concentration, pH, temperature, extract concentration and incubation time based on UV-Visible surface plasmon resonance responses. Optimized conditions were 1.5 mM AgNO₃, pH 11 and 28°C for the aqueous system and 2.0 mM AgNO₃, pH 9 and 50°C for the ethanolic system. FTIR analysis indicated the involvement of hydroxyl/amine, aliphatic C-H, carbonyl/unsaturated and C-O/C-O-C functional groups in nanomaterial formation and surface stabilization. XRD revealed crystalline nanomaterials with average crystallite sizes of 15.20 nm and 31.81 nm for the aqueous and ethanolic preparations, respectively. SEM and TEM revealed predominantly spherical to sub-spherical nanomaterials with varying degrees of aggregation and EDX confirmed elemental silver. SAED demonstrated their polycrystalline nature, with diffraction rings corresponding to the planes of face-centred cubic silver. The aqueous nanomaterials exhibited a zeta potential of -65.5 ± 1.7 mV and a hydrodynamic diameter of 633.7 ± 30.6 nm, consistent with electrostatic stabilization despite moderate aggregation in dispersion. The smaller crystallite size and higher zeta-potential magnitude observed for the aqueous system suggest it as the more promising candidate among the two extracts for downstream functional applications, positioning *H. decipiens* as a sustainable marine resource for green nanomaterial synthesis.

Keywords: *Halophila decipiens*; Green synthesis; Silver nanomaterials; Seagrass; Nanotechnology; Zeta potential.

OP-ESC-48

Theoretical UV Spectral Analysis of Phytochemicals in Traditional Indian Medicinal Herbs (Turmeric and Eucalyptus)

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Abstract

The Indian Knowledge System has introduced numerous medicinal plants with remarkable therapeutic properties. Among them, Turmeric (*Curcuma longa*) and Eucalyptus (*Eucalyptus globulus*) hold significant importance due to their diverse phytoconstituents. This study aims to analyze the phytochemical composition of these plants and explore their medicinal potential using UV-Visible (UV-Vis) spectroscopy. The UV-Vis spectra of key phytoconstituents were simulated using computational tools, and their electronic transitions were studied in detail. A comparative analysis between the simulated spectra and experimentally reported spectra was conducted to evaluate the accuracy of computational spectral predictions. The results demonstrated a strong correlation between simulated and experimental λ max values, validating the efficiency of the software used for UV-Vis spectral analysis. This research not only provides deeper insights into the spectral behavior of bioactive compounds but also reinforces the role of UV-Vis spectroscopy as a powerful tool in medicinal plant research.

Keywords: UV- Visible Spectroscopy, Phytoconstituents, Indian Knowledge System

Unveiling the Bioactive Phytoconstituents of *Vigna angularis*: A Spectroscopic and Antimicrobial Investigation

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Abstract

Vigna angularis (red bean) is a nutritionally rich legume containing diverse bioactive compounds with potential health-promoting properties. The present study investigates the phytochemical composition, spectroscopic characteristics, surface morphology, and antimicrobial potential of *Vigna angularis* extract. Preliminary phytochemical screening was performed to identify major bioactive constituents, including flavonoids, phenolics, tannins, alkaloids, and saponins. Spectroscopic characterization using UV–Diffuse Reflectance Spectroscopy (UV-DRS) and Fourier Transform Infrared (FT-IR) spectroscopy was carried out to evaluate the optical properties and functional groups of the phytoconstituents. The UV-DRS spectrum exhibited a characteristic absorption peak around 298 nm, suggesting the presence of phenolic and flavonoid compounds. The interaction of the extract with magnesium chloride ($MgCl_2$) and zinc chloride ($ZnCl_2$) indicated possible complex formation with metal ions, which may contribute to enhanced biological activity. FT-IR analysis revealed characteristic O–H, C=O, C–O, and N–H functional groups, supporting the presence of diverse phytoconstituents. Surface morphology was examined using Scanning Electron Microscopy (SEM), which revealed irregular and porous particle structures. The antimicrobial activity of the extract was evaluated against selected pathogenic microorganisms, including *Escherichia coli* and *Staphylococcus aureus*, while antifungal activity was assessed against *Aspergillus niger* and *Candida albicans*. The extract showed moderate inhibitory activity, indicating the presence of natural antimicrobial constituents. Overall, the combined phytochemical, spectroscopic, microscopic, and antimicrobial findings demonstrate the biological potential of *Vigna angularis* extract and support its possible application as a natural source for nutraceutical and pharmaceutical development. These findings provide a basis for further investigation of its bioactive constituents and antimicrobial mechanisms for potential future applications.

Key words: *Vigna angularis*, Phytochemical Screening, UV-DRS, FT-IR, SEM Analysis, Antimicrobial Activity, Bioactive Compounds.

OP-ESC-50

The Molecular Structure and Reactivity of Batrachotoxin, A Major Compound Present in Poisonous Frogs

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Abstract

Chemistry plays an important role in the metabolism of living and non-living systems. Although many chemicals found useful in the metabolic reactions occur in human, there are chemicals which are toxic to human and other animals. There are over 170 different species of poisonous frogs which are mainly in Central and South America.¹ They contain extremely toxic compounds in their skin. Nearly more than 800 different alkaloid compounds have been identified in the skin of various frogs. These include *pumiliotoxins*, *histrionicotoxins*, *gephyrotoxins*, and many others. The most well-known of these toxins, is *batrachotoxin*. Batrachotoxin is one of the most toxic alkaloid poisons known. Batrachotoxin kills due to its effect on sodium ion channels in the body. It binds to these channels and jams them open, interfering with nerve transmission and causing muscles to contract. Ultimately, this leads to heart palpitations, then cardiac arrest and death. But the frogs are not affected by these toxic chemicals. Up until now, it is unclear how exactly the newly identified mutation makes it so much harder for batrachotoxin to bind to the channels in these frogs. So far there is no way of preventing batrachotoxin's effect in humans, which would be welcome as there is currently no antidote to the compound. The interesting facts about poisonous frog will be presented.

OP-ESC-51

Green Synthesis, Characterization and Antibacterial Evaluation of Silver Nanoparticles Using *Solena amplexicaulis* Leaf Extract

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Abstract

Methanolic leaf extract of *Solena amplexicaulis* was used in an environmentally friendly method to create silver nanoparticles (AgNPs). The extract-to-silver nitrate ratio, temperature, and reaction time were varied to create three batches. AgNP formation was verified by UV-visible spectroscopy and color change. Characterization techniques included FTIR, SEM, and particle-size analysis. For Batches A, B, and C, absorption maxima were noted at 435, 425, and 410 nm, respectively. Batch C's particles were mostly round or oval in shape, with an average size of 98.1 nm. It demonstrated inhibitory zones of 23, 8, and 31 mm against *S. aureus*, *P. aeruginosa*, and *E. coli*, respectively.

Keywords: Silver nanoparticles; green synthesis; *Solena amplexicaulis*; phytochemicals; characterization; antibacterial activity

Glycerol-Assisted Hydrogen Production Using Bi₂Se₃@g-C₃N₄ Hybrid Electrocatalyst

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Abstract

The development of energy-efficient hydrogen production technologies is essential for advancing sustainable energy systems. In this work, a bismuth selenide–graphitic carbon nitride (Bi₂Se₃@g-C₃N₄) hybrid electrocatalyst is investigated for glycerol-assisted water electrolysis in alkaline media. The integration of Bi₂Se₃ nanosheets with nitrogen-rich g-C₃N₄ provides a synergistic interface that facilitates charge transfer and enhances the accessibility of electrochemically active sites. In 1 M KOH containing 0.2 M glycerol, the Bi₂Se₃@g-C₃N₄ electrode exhibits efficient glycerol oxidation, achieving 10 mA cm⁻² at an anodic potential of 1.30 V vs. RHE, whereas the conventional oxygen evolution reaction requires 1.80 V under identical conditions. On the cathodic side, hydrogen evolution proceeds at an overpotential of 157 mV to attain the same current density. The enhanced electrocatalytic activity is supported by favourable Tafel kinetics and electrochemical impedance characteristics. The hybrid electrode also maintains good catalytic stability during prolonged electrolysis. In addition, glycerol oxidation enables the generation of value-added chemical products while simultaneously facilitating hydrogen production at the cathode. Overall, the Bi₂Se₃@g-C₃N₄ hybrid demonstrates the potential of coupling glycerol oxidation with hydrogen evolution as an energy-efficient approach for sustainable hydrogen production and value-added chemical synthesis.

Keywords: Water splitting, Electrocatalysis, Glycerol oxidation reaction, Hydrogen evolution reaction

Spectroscopic Assessment of Curcumin and Lead Contamination in Turmeric Powder

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Abstract

Turmeric (*Curcuma longa* L.) is an important spice commonly used in food and traditional preparations. Curcumin is one of its major bioactive components, while contamination with heavy metals such as lead can affect the quality and safety of turmeric products. In the present work, turmeric samples were analysed using UV–Visible spectroscopy and Energy Dispersive X-ray Analysis (EDAX) to study the presence of curcuminoids and lead contamination. The UV–Visible spectrum showed a strong absorption band around 420–430 nm, indicating the presence of curcuminoids. The lead-positive sample showed additional absorption bands around 245, 260 and 295 nm, along with a positive colour reaction for lead. EDAX analysis confirmed the presence of Pb in the sample. The results suggest that UV–Visible spectroscopy can be used as a simple preliminary method for screening turmeric samples, while EDAX can be used to confirm the presence of lead. The study emphasizes the importance of checking turmeric products for possible heavy-metal contamination to ensure their quality and safety.

Keywords: Turmeric powder; Curcumin; Lead contamination; UV–Visible spectroscopy; EDAX; Food safety

OP-ESC-54

Vanillin Based Chemosensor for Selective Detection of Mercury Ions in Aqueous Medium

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Abstract

A novel Schiff base ligand derived from vanillin and 2,4-dinitrophenylhydrazine was synthesized and investigated as a fluorescent chemosensor for the selective detection of mercury ions in aqueous medium. The synthesized ligand was characterized using various spectroscopic techniques to confirm its structural and photophysical properties. Fluorescence studies revealed that the Schiff base exhibits remarkable selectivity toward Hg^{2+} ions compared with other competing metal ions such as Co^{2+} , Pb^{2+} , Mg^{2+} , Al^{3+} , K^+ , Na^+ , Ba^{2+} , Bi^{3+} , Ni^{2+} , Cu^{2+} , and Zn^{2+} . A significant fluorescence quenching response was observed upon interaction with Hg^{2+} ions, indicating strong binding affinity between the ligand and the target ion. The detection limit of the sensor was determined to be as low as 10^{-9} M, demonstrating excellent sensitivity. The stability constant of the metal–ligand complex, calculated using the Benesi–Hildebrand method, was found to be $3.7 \times 10^4 \text{ M}^{-1}$. The Stern–Volmer plot showed a linear relationship between F_0/F and quencher concentration, confirming a dynamic quenching mechanism with a quenching constant of 3.4×10^3 . The fluorescence quenching was attributed to a photoinduced electron transfer mechanism. Theoretical calculations supported the experimental findings and provided insight into the interaction mechanism between the ligand and Hg^{2+} ions. These results demonstrate that the synthesized Schiff base ligand acts as an efficient and selective fluorescent chemosensor for mercury ion detection, with potential applications in environmental monitoring and analytical sensing.

Keywords: Schiff base; Vanillin; Mercury ion detection.

Development Of an Eco-Friendly *Gymnema Sylvestre* Extract-Based Corrosion Inhibitor for Mild Steel in Acidic Medium: Experimental and Theoretical Investigations

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Abstract

The corrosion inhibition performance of *Gymnema sylvestre* plant extract for mild steel immersed in 1.0 M H₂SO₄ was investigated using both experimental and theoretical approaches. The phytochemical constituents of the extract were initially characterized by Fourier-transform infrared spectroscopy (FT-IR). Electrochemical measurements, together with theoretical calculations, were subsequently employed to elucidate the inhibition mechanism and adsorption behaviour of the extract on the mild steel surface in an acidic medium. The morphology and surface characteristics of mild steel exposed to the blank and inhibitor-containing solutions were examined using field-emission scanning electron microscopy (FE-SEM) and atomic force microscopy (AFM). The AFM analysis revealed a significant reduction in surface roughness in the presence of the inhibitor, indicating the formation of a protective adsorbed film on the metal surface. Furthermore, UV–Visible spectroscopy provided evidence for the interaction and adsorption of the extract constituents on the steel surface. Contact-angle measurements were also performed to evaluate the wettability of the steel surface. The electrochemical results demonstrated that the inhibition efficiency increased with increasing extract concentration. Electrochemical analysis indicated that the extract acted as a mixed-type inhibitor, affecting both the anodic metal-dissolution and cathodic hydrogen-evolution reactions. The adsorption behaviour of the extract on the mild steel surface was found to follow the Langmuir adsorption isotherm, suggesting the formation of an adsorbed protective layer. The overall results indicated that protonated organic compounds present in the *Gymnema sylvestre* extract possess a strong affinity toward the mild steel surface in acidic conditions.

Keywords: *Gymnema sylvestre*, field emission scanning electron microscopy, sulphuric acid, Langmuir adsorption.

L-cysteine-Functionalized Gelatin composite for Pb (II) Remediation: Adsorption Mechanism and Thermodynamic Insights

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Abstract

Lead (Pb(II)) contamination in aquatic environments poses significant risks to human health and ecosystems, highlighting the need for efficient and sustainable materials for water remediation. In this study, an L-cysteinefunctionalized gelatin composite (L-Cys-Gel) was fabricated via chemical cross-linking as a sustainable adsorbent for Pb(II) removal from aqueous systems. The prepared L-Cys-Gel was characterized by FTIR, XRD, BET, TGA, SEM, and EDX mapping to investigate its structural, surface, morphological, and thermal properties. Batch adsorption experiments were conducted by varying solution pH, adsorbent dosage, contact time, and initial Pb(II) concentration. Under the optimized conditions of pH 8.0, an adsorbent dosage of 30 mg, and an initial Pb(II) concentration of 3 mg L⁻¹, a Pb(II) removal efficiency of 92.84% was achieved within 70 min. Kinetic studies revealed that the adsorption process followed the pseudo-second-order model, suggesting that chemisorption plays a predominant role in Pb(II) uptake. The equilibrium data were well fitted by the Langmuir isotherm, suggesting favorable interactions between Pb(II) ions and the available adsorption sites. Thermodynamic analysis confirmed that the adsorption was spontaneous and endothermic, with enhanced Pb(II) uptake at elevated temperatures. The L-Cys-Gel adsorbent exhibited excellent reusability over five regeneration cycles. The synergistic contribution of thiol, amino, and carboxyl groups within the gelatin matrix highlights the potential of L-Cys-Gel as an effective functional adsorbent for Pb(II) remediation. Overall, this study demonstrates the potential of L-Cys-Gel as a promising and sustainable adsorbent for Pb (II)-contaminated water treatment.

Keywords: Adsorption, L-cysteine, Gelatin, Lead nitrate.

**Nanoscience And Nanotechnology for Energy, Environment and
Biomedical Applications**

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Abstract

Nanoscience and nanotechnology have emerged as promising multidisciplinary fields with significant applications in energy, environmental protection, and biomedical sciences. Nanomaterials exhibit unique physicochemical properties, including high surface area, enhanced catalytic activity, tunable optical and electrical properties, and improved surface reactivity. In the energy sector, nanomaterials are widely explored for solar cells, batteries, supercapacitors, fuel cells, hydrogen production, and photocatalytic energy conversion. In environmental applications, nanoparticles and nanocomposites such as TiO₂, ZnO, Fe₃O₄, graphene-based materials, and carbon quantum dots show great potential for wastewater treatment, pollutant degradation, heavy-metal removal, antimicrobial activity, and air purification. Green-synthesized nanomaterials offer additional advantages by reducing the use of toxic chemicals and promoting sustainable technologies. In biomedical applications, nanotechnology has enabled advances in targeted drug delivery, biosensing, bioimaging, cancer therapy, antimicrobial treatments, and tissue engineering. Despite these advantages, challenges related to toxicity, environmental impact, scalability, cost, and long-term safety need to be carefully addressed. Future research should focus on green synthesis, safe-by-design nanomaterials, sustainable production, and interdisciplinary approaches. The integration of nanotechnology with renewable energy, environmental remediation, biotechnology, and advanced healthcare can contribute significantly to sustainable development and improved quality of life.

Keywords: Nanoscience, Nanotechnology, Nanomaterials, Energy Storage, Photocatalysis, Environmental Remediation, Green Synthesis, Biomedical Applications, Drug Delivery, Biosensors.

Trifunctional Electrocatalyst for Coupling Glucose Electrooxidation Assisted Hydrogen Evolution and Non-enzymatic Glucose Sensing

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Abstract

The selective electro-oxidation of organic molecules coupled with the hydrogen production is emerging as an energy-efficient approach to produce renewable energy. This study reports a trifunctional nickel phosphide based Ni_{12}P_5 catalyst to address glucose oxidation reaction (GOR) and non-enzymatic glucose detection, coupling with efficient hydrogen production. Binder-free electroless plating is used to produce an even layer of Ni_{12}P_5 catalyst on flexible and sustainable polyester cotton fabric. Precise glucose detection plays a critical role in clinical diagnostics, diabetes management, and real-time biochemical monitoring. Ni_{12}P_5 fabric electrode demonstrated excellent selectivity and high sensitivity for non-enzymatic glucose detection down to 50 μM glucose concentration. Systematic electrochemical investigations performed with various glucose concentrations confirm concentration-dependent electro-oxidation of glucose. In situ Raman spectroscopy confirms the dynamic transformation of NiOOH species, which act as the active sites for GOR. In short, this study provides an integrated concept of sensing and renewable energy generation using an eco-friendly and cost-effective fabric supported electrodes.

Keywords: Nickle phosphide, Non-enzymatic glucose sensing, Glucose oxidation, Flexible electrode

Application of Recyclable Nano Catalyst for Biodiesel Production: A Review

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Abstract

Biodiesel production commonly relies on homogeneous catalysts, which can provide high conversion but create difficulties in catalyst separation, product purification, wastewater generation, and catalyst recovery. Recyclable nanocatalysts have emerged as promising alternatives because their high surface area, tunable surface chemistry, and potential for magnetic or filtration-based recovery can improve process efficiency and sustainability. This review critically examines recent developments in recyclable nanocatalysts for biodiesel synthesis, including metal-oxide, carbon-based, biomass-derived, supported, magnetic, and nanobiocatalytic systems. Studies were evaluated with respect to catalyst preparation, structural and surface characteristics, feedstock compatibility, reaction conditions, biodiesel yield, recovery techniques, reusability, deactivation, environmental performance, and economic feasibility. It demonstrates that nanostructured catalysts can enhance mass transfer and promote esterification and transesterification, often achieving high conversion under comparatively mild conditions. Magnetic nanocatalysts facilitate rapid separation, while supported and biomass-derived materials can reduce catalyst loss and production costs. Many systems retain substantial activity over several reaction cycles; however, performance may decline because of active-site poisoning, leaching, fouling, sintering, and incomplete recovery. Despite their potential to reduce chemical consumption, wastewater formation, and downstream processing requirements, large-scale application remains limited by preparation cost, nanoparticle agglomeration, uncertain long-term stability, catalyst contamination of biodiesel, and insufficient life-cycle and toxicity assessments. Future research should prioritize standardized recyclability testing, scalable synthesis, safer-by-design materials, continuous reactors, and techno-economic and environmental validation. Recyclable nanocatalysts therefore represent a significant route toward cleaner, more efficient, and potentially circular biodiesel production.

Keywords: Reusable, Catalytic activity, Biofuel, Circular economy

From PET Waste to Formic Acid and Hydrogen: Nb-NiCoS for Energy-Efficient Electro-Upcycling

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Abstract

Electrocatalytic polyethylene terephthalate (PET) upcycling coupled with green hydrogen production offers an energy-efficient route for plastic waste valorization. Herein, Nb-incorporated NiCoS electrocatalysts are synthesized on nickel foam via a one-step chemical bath deposition route for industrial-current-density PET electro-upcycling. Nb incorporation modulates the electronic structure and morphology of NiCoS, producing defect-rich vertically interconnected nanosheets with abundant electrochemically dynamic $\text{Ni}^{3+}/\text{Co}^{3+}$ active sites. The optimized electronic structure promotes reconstruction into active NiOOH/CoOOH species, resulting in enhanced performance toward the hydrogen evolution reaction (HER), oxygen evolution reaction (OER), ethylene glycol oxidation reaction (EGOR), and PET hydrolysate oxidation reaction (POR). Nb-NiCoS requires 1.32 and 1.34 V vs RHE to achieve 100 mA cm^{-2} for EGOR and POR, respectively, significantly lower than OER (1.52 V vs RHE). Mechanistic analysis reveals an indirect oxy-hydroxide-mediated oxidation pathway, enabling selective conversion of PET-derived EG into formic acid with a Faradaic efficiency of 93.1% and a production rate of $2.30 \text{ mmol h}^{-1} \text{ cm}^{-2}$ at 200 mA cm^{-2} . Coupling PET electro-upcycling with hydrogen production reduces the energy consumption from 4.49 to 3.52 kWh Nm^{-3} under industrial alkaline conditions, enabling energy saving of 21.3%, highlighting a scalable strategy for simultaneous plastic waste valorization and hydrogen production.

Keywords: Electro-upcycling of PET plastic; ethylene glycol oxidation reaction; hydrogen evolution reaction; in-situ operando Raman spectroscopy.

OP-ESC-61

Microwave-Assisted Synthesis of Magnetic Activated Carbon from Cabbage Leaf Waste for Efficient Chromium Removal from Tannery Wastewater

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Abstract

Cabbage leaf waste was utilized as a sustainable biomass precursor for the rapid synthesis of magnetic activated carbon using a microwave-assisted method. The synthesised magnetic activated carbon was characterized using FTIR, XRD, HRTEM–EDX, BET surface area analysis, and other relevant techniques to investigate its structural, morphological, textural, elemental, and magnetic properties. The adsorbent was investigated for the removal of toxic metal from tannery wastewater, with particular emphasis on chromium contamination. Adsorption efficiency of the magnetic activated carbon was examined with various parameters, including adsorbent dosage, chromium ion concentration, contact time, and temperature, to determine the optimum removal conditions. The adsorption mechanism was further examined using kinetic and isotherm models. Chromium removal efficiency was about 87%. Additionally, the adsorption isotherm and kinetics magnetic activated carbon conformed to the Langmuir adsorption isotherm ($R^2 = 0.991$) and quasi-second-order kinetic model ($R^2 = 0.994$). The magnetic activated carbon exhibited promising potential for efficient toxic metal removal owing to its porous structure and surface-active functional groups. Moreover, its magnetic nature enables facile recovery from treated water, improving its practical applicability. This microwave-assisted approach provides a simple and sustainable strategy for converting cabbage leaf waste into a value-added adsorbent for wastewater treatment and environmental remediation.

Keywords: Magnetic activated carbon, Fe₃O₄ nanoparticles, Adsorption, Sustainable sensor

Photocatalytic Performance of Psidium guajava-Derived Cu-Doped ZnO Nanoparticles toward Congo Red Dye Degradation

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Abstract

A sustainable plant-mediated approach was employed to synthesize Copper-doped Zinc Oxide (Cu–ZnO) nanoparticles using *Psidium guajava* leaf extract with their photocatalytic potential assessed through the degradation of Congo red (CR). The synthesized Cu–ZnO nanoparticles were characterized using Fourier-transform infrared spectroscopy (FTIR), UV–visible spectroscopy, scanning electron microscopy (SEM) and photoluminescence (PL) spectroscopy to investigate their functional groups, optical absorption, surface morphology and charge-carrier recombination behavior. Cu incorporation into ZnO induced changes in its optical absorption, electronic properties and surface morphology as evidenced by the UV– visible, photoluminescence and SEM analyses. The photocatalytic activity was evaluated by monitoring the degradation of Congo red under light irradiation and the degradation kinetics were analyzed to determine the photocatalytic efficiency. Cu– ZnO demonstrated enhanced photocatalytic degradation of Congo red which may be associated with improved light absorption and reduced photogenerated electron–hole recombination resulting from Cu incorporation [1]. The use of *P. guajava* leaf extract offers a simple and environmentally favorable approach to synthesize nanoparticle while minimizing the use of conventional chemical reagents. Overall, the synthesized Cu–ZnO nanoparticles demonstrate promising potential for the photocatalytic remediation of Congo red-containing dye wastewater.

Keywords: Green synthesis, Congo red, *Psidium Guajava*, Nanoparticles, Cu-Doped ZnO

Engineering Metal Centres in BTC-based Metal-Organic Frameworks for Electrochemical CO₂ Reduction

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Abstract

Electrochemical CO₂ reduction reaction (eCO₂RR) offers a promising route for converting CO₂ into value-added chemicals under mild operating conditions, but the development of efficient and selective metal-organic framework (MOF) electrocatalysts remains challenging. Herein, we synthesized Bi-, Ce-, and Zn-based metal-organic frameworks coordinated with benzene-1,3,5-tricarboxylic acid (BTC) ligands via a facile room-temperature route and systematically investigated them as electrocatalysts for eCO₂RR. pXRD, solid-state NMR spectroscopy, FTIR and Raman spectroscopy, FE-SEM, TEM and HR-TEM, XPS, and TG analysis were used to comprehensively elucidate the structural and chemical features of the resulting frameworks. The three MOFs exhibited distinct electrochemical responses toward CO₂ reduction. Among them, Bi-BTC showed a lower onset potential and delivered the highest current density, reaching -27.94 mA cm⁻² at -1.10 VRHE. Electrochemical impedance and kinetic analyses further revealed a relatively low charge-transfer resistance of 102.8 Ω and a Tafel slope of 147 mV dec⁻¹ for Bi-BTC, indicating more favorable interfacial charge-transfer and reaction kinetics compared with the Ce- and Zn-based analogues. Preliminary product analysis by HPLC further established a metal-dependent trend in formic acid formation, with Bi-BTC exhibiting the highest formic acid production, followed by Zn-BTC and Ce-BTC frameworks. These results demonstrate that variation of the metal node within structurally related BTC frameworks can substantially influence their electrochemical CO₂-reduction behavior and provide a comparative platform for correlating MOF structure and metal-center chemistry with catalytic performance.

Keywords: Electrochemical CO₂ reduction; Metal-organic frameworks (MOFs); BTC ligand; Formic Acid; Value-added product;

OP-ESC-64

From Plant Waste to Smart Packaging: Banana Bract and Flaxseed-Reinforced *Colocasia* Starch Biocomposites

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Abstract

The increasing demand for sustainable alternatives to conventional petroleum-based plastics has stimulated significant interest in biodegradable and bio-based packaging materials. The present study focuses on the development of sustainable antimicrobial packaging films based on *Colocasia* starch, banana bract extract and flaxseed gel. *Colocasia* starch serves as the primary biodegradable polymer matrix, while flaxseed gel acts as a natural film-forming and reinforcing component. Banana bract extract, a renewable agricultural by-product rich in bioactive phytochemicals, is incorporated to impart potential antimicrobial and antioxidant properties to the biocomposite films. The prepared films will be evaluated for their physicochemical, structural, mechanical, thermal, barrier and biodegradation properties using techniques such as FT-IR spectroscopy, UV–Visible spectroscopy, XRD, SEM and thermal analysis. Their antimicrobial performance will be assessed against selected foodborne and pathogenic microorganisms, while antioxidant activity may be evaluated using suitable radical-scavenging assays. The influence of banana bract extract and flaxseed gel concentration on film morphology, tensile strength, flexibility, water resistance and antimicrobial efficiency will also be investigated. The incorporation of these natural components is expected to improve the functional performance of *Colocasia*-starch-based films while reducing dependence on synthetic packaging materials. This work demonstrates a promising circular-bioeconomy approach for converting agricultural biomass into value-added, biodegradable and potentially active food-packaging materials, with potential applications in sustainable food preservation and environmentally friendly packaging.

Keywords: *Colocasia* starch, Banana bract extract, Flaxseed gel, Biocomposite films, Sustainable packaging, Antimicrobial activity, Antioxidant activity

OP-ESC-65

Development of Sustainable Fe-MOF/Neem Gum–Alginate Composite

Beads for Efficient Adsorption Applications

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Abstract

In the present study, an iron-based metal–organic framework (Fe-MOF) was synthesized by a solvothermal method using ferric nitrate nonahydrate $[\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}]$ as the metal precursor and 2-aminoterephthalic acid ($\text{NH}_2\text{-BDC}$) as the organic linker in a mixed solvent system of N,N-dimethylformamide (DMF), distilled water, and acetic acid. To improve the handling, recovery, and practical applicability of the resulting adsorbent, the Fe-MOF/neem gum composite was immobilized in sodium alginate to form bead-shaped materials. The synthesized Fe-MOF and Fe-MOF/neem gum–alginate beads were characterized using Fourier-transform infrared spectroscopy (FTIR), UV–visible spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM). FTIR analysis was used to identify the characteristic functional groups and possible interactions between the Fe-MOF, neem gum, and sodium alginate. UV–visible spectroscopy provided information regarding the optical absorption characteristics, while XRD analysis was employed to investigate the crystalline structure of the synthesized material. SEM analysis revealed the surface morphology and bead structure of the composite adsorbent and DLS. The combination of a porous Fe-MOF framework with the functional groups of neem gum and the convenient bead form provided by sodium alginate offers a promising sustainable platform for environmental remediation applications, particularly for the removal of contaminants from aqueous systems.

Keywords: 1, Metal–organic frameworks 2, Heavy metal removal 3, Fe-MOF 4, Solvothermal

Sustainable Corrosion Protection of Mild Steel in Hydrochloric Acid Using Hybanthus Enneaspermus leaf Extract: Mechanistic Insights from Adsorption and Electrochemical Studies

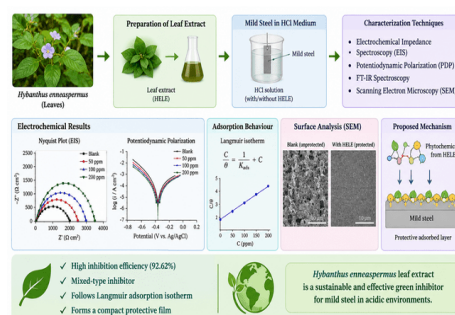
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Abstract

Natural plant extracts have emerged as promising green alternatives to conventional corrosion inhibitors owing to their abundance, biodegradability, renewability, low toxicity, and environmental compatibility. In this study, the corrosion inhibition performance of *Hybanthus enneaspermus* leaf extract (HELE) for mild steel in an acidic medium was systematically evaluated using electrochemical and surface characterization techniques¹. Electrochemical impedance spectroscopy (EIS) revealed a maximum inhibition efficiency (IE%) of 92.62% at the optimum concentration of HELE. The impedance spectra were well described by an equivalent electrical circuit comprising two time constants, corresponding to the charge-transfer process and the formation of a protective surface film. Increasing the HELE concentration enhanced the charge-transfer resistance (R_{ct}) while decreasing the double-layer capacitance (C_{dl}), confirming the development of an adsorbed protective layer on the mild steel surface. Potentiodynamic polarization studies further established that HELE acts as a mixed-type inhibitor by suppressing both anodic metal dissolution and cathodic reactions. The adsorption of phytochemical constituents presents in HELE onto the mild steel surface was found to obey the Langmuir adsorption isotherm, suggesting favorable surface coverage by the inhibitor molecules. FT-IR analysis identified electron-rich functional groups associated with the adsorption of phytoconstituents onto the metal surface. Furthermore, SEM characterization revealed a relatively smooth and compact protective film on the inhibited mild steel surface compared with the uninhibited specimen². These findings demonstrate the potential of *Hybanthus enneaspermus* leaf extract as an environmentally benign and effective corrosion inhibitor for mild steel in acidic environments.



Keywords: Corrosion, *Hybanthus enneaspermus*, Adsorption, Impedance, Polarization, SEM.

**Histidine-Modified Poly N-Methyl aniline for Sustainable Corrosion
Mitigation of Mild Steel in Acidic Environment**

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Abstract

Poly aniline is an attractive material for corrosion inhibition studies. In this study, poly N-methyl aniline doped with Histidine and explored for their inhibitive action of mild steel corrosion in 0.5M Sulphuric acid. The doped polymer was evaluated using weight loss method, polarization studies and electrochemical impedance studies. The doped polymer exhibited maximum efficiency of 91.21% at the concentration 230 ppm. The inhibitor efficiency of doped increased at 3 hours of immersion followed by a decrease, and an increase at 24 hours of immersion. Potentiodynamic polarization studies indicate the polymer as mixed inhibitors. The impedance measurements and polarization studies were comparable with the weight loss studies. The synergistic action of poly aniline and doped polymer was confirmed by the synergistic parameter calculation. The changes occurred in the electrolytic solution after the immersion of mild steel samples for 6 h of immersion period was determined by Atomic absorption spectroscopy and UV-visible spectroscopic studies. The results provide some preliminary information about the complex formation in the solution phase and also the protective layer formation on the metal surface. The protective layer is characterized using Scanning electron microscopy and EDAX analysis.

Keywords: Poly aniline, Doped polymer, Histidine, mild steel, SEM

Structure–Property Correlations in *Psidium guajava*-Mediated Fe–Pb Bimetal Oxide Nanoparticles: Structural, Morphological and Functional Investigations

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Abstract

The present study focuses on the green synthesis and characterization of Fe–Pb bimetal oxide nanoparticles using *Psidium guajava* plant extract as a sustainable biological source. The naturally occurring phytochemicals present in *P. guajava* extract facilitate the formation and stabilization of the Fe–Pb bimetal oxide nanoparticles, providing an eco-friendly alternative to conventional chemical synthesis methods. The synthesized nanoparticles were systematically investigated to understand their structural, functional, morphological and elemental characteristics. Fouriertransform infrared (FTIR) spectroscopy was employed to identify the functional groups associated with the phytochemicals involved in the synthesis and the characteristic metal–oxygen bonds. X-ray diffraction (XRD) analysis was used to investigate the crystalline structure and phase characteristics of the synthesized material. Scanning electron microscopy (SEM) was employed to examine the surface morphology and particle distribution, while energy-dispersive X-ray spectroscopy (EDX) was utilized to confirm the elemental composition of iron and lead. The incorporation of two metal components within the oxide system is expected to impart distinctive physicochemical characteristics compared with their corresponding individual metal oxides. The *Psidium guajava*mediated green synthesis approach provides a sustainable and environmentally friendly route for the preparation of Fe–Pb bimetal oxide nanoparticles. The synthesized material offers a promising platform for further investigations in areas such as catalysis, environmental remediation, sensing and other emerging nanotechnology applications.

Keywords: *Psidium guajava*, Green synthesis, Fe–Pb bimetal oxide nanoparticles, XRD, FTIR, SEM, EDX, Nanotechnology.

DFT-Based Investigation of Organic Corrosion Inhibitors and their Adsorption on Metal Surfaces

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Abstract

Quantum chemical calculations for the adsorption and inhibition mechanism that relate the Density functional theory (DFT) has been used to analyse the characteristics of the inhibitor/surface mechanism and to describe the structural 4-(pyridin-2yl)-N-p-tolylpiperazine-1-carboxamide (PTC) of the inhibitor in the corrosion process. DFT can be used to design corrosion inhibitor to prevent corrosion on mild steel. The optimized molecular structure E_{HOMO} , E_{LUMO} and MEP of PTC. The 3D structure and frontier molecular orbital calculated at density functional theory (DFT) level of approximation. DFT is the simplest way to study the molecular structure and behavior of corrosion inhibitors. Some of the quantum chemical parameters such as dipole moment, highest occupied molecular orbital (E_{HOMO}), lowest occupied molecular orbital E_{LUMO} , energy gap (ΔE), chemical hardness (η), softness (σ), absolute electronegativity (χ) and electrophilicity (ω) of the PTC models were calculated. Higher values of E_{HOMO} are an indication of the greater ease of donating electrons to the unoccupied d orbital of metal, and the higher the corrosion inhibition efficiency.

Keywords: Density functional theory (DFT), dipole moment, E_{HOMO} , E_{LUMO}

Development of pH-Responsive Anthocyanin-Loaded Starch–Chitosan Biodegradable Films for Intelligent Food Freshness Monitoring

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Abstract

The present study reports the development of a biodegradable and pH-responsive films based on Oat starch/Chitosan matrix along with anthocyanins from grape peel and black rice extracts for food freshness monitoring. FTIR analysis confirmed the characteristic functional groups and interactions within the polymeric matrix, while TGA demonstrated the thermal behavior and stability of the developed films. SEM analysis revealed the surface morphology and structural characteristics of the film. The developed films were further evaluated for solubility, swelling index, biodegradation, water vapor permeability, moisture content, and pH responsiveness. The films exhibited distinct color changes under different pH conditions, demonstrating their potential to serve as visual freshness indicators. Antimicrobial studies further demonstrated the functional activity of the developed films against the tested microorganisms. The practical applicability of the films was investigated using cucumber, grapes, and bread as model food products. Thus, the prepared film was found to be efficient for food packaging applications.

Keywords: Oat starch, Chitosan, intelligent film, food freshness, antimicrobial activity

Magnetic Biosorbents: A Systematic Review

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Abstract

The contamination of water bodies by heavy metals, dyes, and emerging organic pollutants poses severe risks to environmental and public health. Conventional remediation techniques such as precipitation, ion exchange, and membrane filtration are often limited by high costs, secondary waste generation, and poor efficiency at low pollutant concentrations. Biosorption using agricultural waste, algae, fungi, and bacteria has emerged as a sustainable and cost-effective alternative; however, practical application is hindered by difficulties in separating the biomass from treated water. This review addresses the critical challenge of postsorption separation by evaluating magnetic biosorbents, biomaterials modified with magnetic nanoparticles that enable rapid, simple recovery using an external magnetic field. Comprehensive findings reveal that magnetic modification enhances sorption capacity by 2040% compared to native biomass, improves reusability over multiple cycles (up to 85% efficiency retained after five cycles), and allows efficient operation across a wide pH range (39). The most effective matrices include magnetic chitosan, magnetic cellulose, and magnetized algal biomass, with maximum adsorption capacities reaching 200-500 mg g⁻¹ for heavy metals. Major challenges include nanoparticle leaching, synthesis cost, and scale-up feasibility. This concludes that magnetic biosorbents represent a transformative platform for next-generation water treatment, offering a synergistic combination of high removal efficiency, facile separation, and environmental compatibility. However, inconsistent testing protocols, nanoparticle aggregation, metal leaching, declining capacity during regeneration, complex wastewater matrices, and limited pilot-scale and life-cycle assessments continue to restrict practical deployment. Future research should emphasize standardized evaluation, scalable lowimpact synthesis, magnetic-phase stability, contaminant recovery, and safe management of spent materials. Magnetic biosorbents offer a promising route for circular, efficient, and adaptable water purification when performance and environmental risks are assessed together.

Keywords: Water Treatment, Heavy Metal Removal, Magnetic Nanoparticles, Sustainable Remediation

OP-ESC-72

Carbon Dot Incorporated Films for Enhanced Seed Germination

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Abstract

Carbon dots (CDs) are zero-dimensional carbon-based nanomaterials that has excellent fluorescence, photostability, and optical properties. They are widely used for sensing, photocatalysis, photocatalysis, and environmental applications. CDs can also be used as sustainable source of nutrients required for seed germination and growth due to their environmental friendliness and ease of synthesis. This work presents a sustainable, easily degradable, carbon-dot (CDs) incorporated seed pouch. In this approach, CDs were prepared from sustainable sources like banana peel (BPCDs) and rice husk (RHCDs) by hydrothermal method. These CDs were individually incorporated into films that were cast with Polyvinyl alcohol (PVA). A pouch was made from the film and green gram seeds were placed inside the pouch. It was planted in the soil and was kept under uniform environmental conditions. An evident elongation in the leaf size, shoot length, and an increase in the density of the roots were observed, compared to the control samples which did not use the pouch. This indicates that the CDs incorporated seed pouches are environmentally friendly and boost the development of a healthier plant.

A Multi-criteria Decision-Making framework using Neutrosophic soft set similarity measure for Regional Weather Pattern Analysis

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Abstract

Weather pattern analysis across multiple geographic regions requires handling incomplete, uncertain, and imprecise meteorological data — a challenge classical statistical methods often address inadequately. This paper proposes a Multi-Criteria Decision-Making (MCDM) framework based on Neutrosophic Soft Set (NSS) similarity measures to analyze and compare regional weather patterns across five districts using five meteorological parameters (temperature, humidity, rainfall, wind speed, and surface pressure) sourced from NASA POWER data. Each district-parameter observation is transformed into a neutrosophic triple (Truth, Indeterminacy, Falsity) via min-max normalization, capturing not only the degree to which a condition holds but also the inherent uncertainty in classification. A weighted similarity measure, incorporating district-specific importance weights, is applied to construct a pairwise similarity matrix across districts and across a five-year period (2021–2025), enabling identification of climatically similar regions, anomalous years, and the most volatile meteorological parameters. The α -similarity threshold is used to formally classify district-pairs and year-pairs as similar or dissimilar. Results demonstrate that the proposed framework provides a robust, interpretable, and mathematically grounded decision-support tool for regional climate comparison, outperforming simple correlation-based methods in handling data uncertainty. The findings offer practical value for agricultural planning, water resource management, and regional policy-making in climate-sensitive areas.

Keywords: Neutrosophic Soft Set; Similarity Measure; Multi-Criteria Decision-Making; Weather Pattern Analysis; NASA POWER; Regional Climate Comparison

Photocatalytic Nanomaterials for Sustainable Waste Water Treatment: Mechanisms, Applications & Future Perspectives

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Abstract

Photocatalysis is an emerging and sustainable approach for wastewater treatment, particularly for the degradation of persistent organic pollutants, dyes, pharmaceuticals and other contaminants. Semiconductor nanomaterials such as titanium dioxide (TiO₂), zinc oxide (ZnO) and graphitic carbon nitride (g-C₃N₄) can utilize light energy to generate electron-hole pairs and reactive oxygen species responsible for pollutant degradation. However, limited visible-light absorption, charge recombination and difficulty in catalyst recovery can restrict their practical application. To review the potential of semiconductor-based photocatalytic nanomaterials for sustainable wastewater treatment, with emphasis on photocatalytic mechanisms, pollutant degradation and strategies for improving treatment efficiency. A review of available scientific literature was carried out using PubMed and Google Scholar, with emphasis on research studies and review articles concerning photocatalytic wastewater treatment and semiconductor nanomaterials. Studies involving TiO₂, ZnO, g-C₃N₄ and heterojunction - based photocatalysts were considered. Factors influencing photocatalytic performance, including light intensity, pH, catalyst concentration and pollutant concentration, were also examined. The reviewed evidence indicates that photocatalytic nanomaterials can effectively degrade various organic pollutants and dyes through reactive oxygen species generated under light irradiation. Doping, surface modification and heterojunction formation can improve visible-light absorption and reduce electron-hole recombination, thereby enhancing photocatalytic activity. However, catalyst recovery, stability, cost and large-scale application remain important challenges. Photocatalytic nanotechnology represents a promising sustainable strategy for wastewater remediation. Development of stable, recyclable and visible-light-responsive photocatalysts could improve their practical and industrial applicability.

Keywords: Photocatalysis; Nanomaterials; Wastewater treatment; Semiconductor photocatalysts; Sustainable remediation.

Nanotechnology In Agriculture and Food: Emerging Approaches for Sustainable Production and Food Safety

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Abstract

Nanotechnology is emerging as a transformative platform for advancing sustainable agriculture, precision crop management, and food safety. The distinctive physicochemical, interfacial, catalytic, and antimicrobial properties of engineered nanomaterials facilitate targeted delivery, controlled release, real-time sensing, and enhanced protection across the agricultural and food value chains. This review critically examines recent advances in nano-enabled agriculture and food technologies, focusing on nanofertilizers, nanopesticides, nanostimulants, nanosensors, nanobiosensors, and functional nanocomposite packaging. Relevant peer-reviewed literature published through scientific databases, including PubMed, PubMed Central, and other scholarly sources, was evaluated to identify emerging applications, technological advantages, and safety considerations. Recent evidence indicates that nanoformulated fertilizers and agrochemicals can improve nutrient-use efficiency and enable controlled delivery of active ingredients, thereby supporting precision input management and potentially reducing agricultural losses. Nanosensors and nanobiosensors offer sensitive and rapid detection of plant pathogens, phytochemicals, environmental contaminants, toxins, and indicators of crop and soil health. In food systems, nanostructured and nanocomposite materials can improve mechanical and barrier properties, provide antimicrobial activity, facilitate active and intelligent packaging, and contribute to preservation and shelf-life extension. Nevertheless, nanoparticle transformation, environmental persistence, plant uptake, bioaccumulation, potential toxicity, human exposure, regulatory harmonization, and consumer acceptance remain critical challenges. Overall, nanotechnology represents a promising enabling technology for resource-efficient agriculture and safer food systems; however, its sustainable translation requires standardized risk assessment, life-cycle evaluation, regulatory oversight, and long-term environmental and toxicological investigations.

Keywords: Nanotechnology; Nanofertilizers; Nanopesticides; Nanostimulants; Nanosensors; Food Safety; Nanocomposite Packaging; Sustainable Agriculture.

Green Human Resource Practices and Environmental Sustainability: Evidence from Organizations in Delhi NCR

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Abstract

Green Human Resource Management (GHRM) integrates environmental considerations into human resource policies and practices to encourage employees to participate in organizational sustainability initiatives. Although the existing literature has established an association between GHRM and environmental performance, empirical evidence examining how specific green workplace practices contribute to environmental sustainability within Indian organizations remains limited. This study therefore investigates the relationship between GHRM practices and environmental sustainability among organizations in the Delhi National Capital Region (NCR). The study adopts a quantitative, cross-sectional research design. Primary data were collected from employees and managers through a structured questionnaire using a five-point Likert scale. Of the 300 respondents targeted, 270 responses were received, of which 252 were verified as valid and complete for statistical analysis. The study examines key GHRM dimensions, including green recruitment and staffing, green training and development, employee engagement, green performance management, compensation, organizational communication, and leadership. Data were analyzed using SPSS and Microsoft Excel through descriptive statistics, Cronbach's alpha reliability analysis, Pearson correlation, and regression analysis. The study examines whether GHRM practices are significantly associated with environmental sustainability and considers how environmentally oriented HR practices can support green workplace behaviour and organizational sustainability. The findings indicate a positive association between GHRM practices and environmental sustainability, with a reported Pearson correlation coefficient of $r = 0.477$. The regression analysis also reports a positive and statistically significant coefficient for GHRM practices ($B = 0.322$, $p < 0.001$). The study provides empirical evidence from the Delhi NCR context and highlights the relevance of integrating environmental objectives into HR strategies to support employee participation in organizational sustainability initiatives.

Keywords: Green Human Resource Management; Environmental Sustainability; Green Workplace Practices; Green Employee Behaviour; Sustainable HRM; Delhi NCR

OP-ESC-77

Valorisation Of Fruit Peel Waste Through Green Synthesis of Bioactive Silver Nanoparticles

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Abstract

The present study focuses on the green synthesis of silver nanoparticles (AgNPs) using a polyherbal aqueous extract of passion fruit (*Passiflora edulis*), avocado (*Persea americana*), and dragon fruit (*Hylocereus undatus*), and the evaluation of their phytochemical and biological properties. Qualitative phytochemical screening confirmed the presence of alkaloids, carbohydrates, phenols, flavonoids, proteins, and saponins, while quantitative analysis revealed significant total phenolic and flavonoid contents. The antioxidant potential assessed by DPPH assay demonstrated strong free radical scavenging activity. Furthermore, the extract exhibited notable anti-inflammatory and antidiabetic activities, indicating its therapeutic potential. The synthesized AgNPs were characterized using FTIR analysis, which confirmed the involvement of functional groups such as hydroxyl, carbonyl, and amine groups responsible for the reduction and stabilization of nanoparticles. These findings suggest that the phytochemicals present in the polyherbal extract act as effective reducing and capping agents during nanoparticle synthesis. Overall, the study highlights an eco-friendly, cost-effective approach for AgNP synthesis with promising biomedical applications.

Keywords: Polyherbal extract, Silver nanoparticles, Green synthesis, FTIR, Phenolic compounds.

Z.E.N.I.T.H. – Zwitterionic Engineered Nanoparticle-Infused Tea Harvester

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Abstract

Global water scarcity necessitates the development of sustainable, decentralized atmospheric water harvesting and purification systems. However, current solar-driven evaporators frequently fail due to severe salt accumulation (fouling) and produce purely distilled water devoid of essential dietary minerals. To address these critical limitations, this paper introduces Z.E.N.I.T.H. (Zwitterionic Engineered Nanoparticle-Infused Tea Harvester), a novel, autonomous, solar-powered water recovery system leveraging upcycled agricultural biomass. The core functional matrix utilizes spent *Camellia sinensis* (tea) leaves, transforming zero-cost cellulosic waste into a highly porous, photothermal bio-scaffold optimized for rapid solar evaporation and atmospheric moisture capture. To overcome scaling constraints in high-salinity environments, the tea hydrogel matrix is engineered with a surface-grafted zwitterionic polymer network. This specialized layer generates a robust hydration shell that physically repels inorganic salts and organic foulants, ensuring long-term, self-cleaning durability without synthetic chemical maintenance. Crucially, Z.E.N.I.T.H. bridges the gap between basic water extraction and human health via active nanotechnological mineralization. As the condensed, purified water flows through the final collection interface, embedded controlled-release nano-minerals—specifically engineered calcium and magnesium nanospheres—fortify the yield. This process actively converts the distilled output into nutritionally functional, potable drinking water. Powered autonomously by integrated solar photovoltaics, the system is designed for continuous, off-grid operation. By synergizing advanced sustainable materials engineering, nanoparticle integration, and zero-waste upcycling, Z.E.N.I.T.H. establishes a highly scalable, low-maintenance framework for generating remineralized, safe drinking water in remote and resource-limited environments.

Keywords: Atmospheric Water Harvesting, Solar Evaporation, Nanoparticle Mineralization, Zwitterionic Polymers, Anti-Fouling, Biomass Upcycling.

Rhizo-Methane Bridge: A Nanostructured Porous Root-Zone Biointerface for Methane Mitigation in Flooded Rice Fields

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Abstract

Rice cultivation under flooded conditions is a significant agricultural source of methane (CH_4), a potent greenhouse gas. Waterlogged soils create anaerobic conditions that favor methanogenic microorganisms, while rice plants transport oxygen to the root zone through specialized aerenchyma tissues. This naturally occurring oxygen–methane interface can support methane-oxidizing microorganisms (methanotrophs). The proposed RHIZO-METHANE BRIDGE aims to enhance this natural process using a strategically distributed porous biointerface incorporating cellulose nanofibers (CNF) as a nanostructured scaffold. The CNF-based porous structure is designed to provide a high-surface-area environment for microbial attachment and biofilm development while facilitating localized gas exchange between methane and oxygen. Rather than applying the material to individual plants, the system will be investigated using hotspot- or strip-based placement within the rice root zone, providing a potentially scalable approach for flooded-field application. Controlled rice–soil microcosm experiments will evaluate methane emission, soil oxygen concentration, redox potential, methanotrophic activity, microbial colonization, and plant growth. The study integrates rice physiology, soil microbiology, nanostructured biomaterials, and environmental biotechnology to investigate whether a CNF-based porous biointerface can enhance native methane oxidation and reduce methane transport to the atmosphere. The proposed approach provides a novel framework for engineering the rice root–soil–microbe interface for sustainable methane mitigation.

Keywords: Rice, Methane mitigation, Aerenchyma, Methanotrophs, Rhizosphere, Porous biointerface, Nanotechnology

Green Synthesis of Titanium Nanoparticles from Citrus Medica Leaves with Significant Anti-Ageing Efficacy

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Abstract

The biosynthesis of Titanium nanoparticles is being studied for its possible application in the environmentally friendly development of new technology. Nanoparticles are typically created using a variety of chemical methods that are not environment friendly. The plant Citrus medica leaves was used in the synthesis of titanium nanoparticles by green method. Within one hour of treating a 1mM titanium oxide (TiO₂) aqueous solution with the leaf extract of citrus medica the titanium oxide nanoparticles could be synthesised. Fourier Transform Infrared spectroscopy (FTIR), UV-Visible spectroscopy and X-ray Diffraction (XRD) were used to characterise these nanoparticles. The face centred cubic crystal structure of these nanostructures was confirmed by X- ray diffraction (XRD) results. The anti-ageing analysis revealed that the synthesised titanium oxide nanoparticles had a higher percentage of inhibition. The results of the titanium nanoparticles synthesized using the leaves of Citrus medica exhibited a maximum of 78% inhibition for anti- collagenase and for the anti-elastase model the inhibition is about 70%.

Keywords: Green synthesis, Titanium oxide nanoparticles (TiO₂ NPs), Citrus medica leaves, Anti-ageing activity.

Isolation, Characterization and Storage stability of Plant-Derived Extracellular Vesicles from *Colocasia esculenta* (L.) Schott leaves as Potential Nanoplatfoms

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Abstract

Colocasia esculenta (Taro) is an edible plant whose leaves are rich in proteins, dietary fibre and micronutrients with promising anticancer, antioxidant and anti-inflammatory properties. Meanwhile, Plant-derived Extracellular vesicles are nano-sized lipid bilayer vesicles, as natural carriers of therapeutic relevant bioactive molecules, however, their occurrence in *C. esculenta* leaves remains unexplored. The study focused on isolation and characterization of extracellular vesicles from *C. esculenta* leaves (CELEVs) and assess their storage stability under different temperatures. CELEVs were isolated by differential Ultra-centrifugation and characterized by Transmission Electron Microscopy (TEM), Dynamic Light Scattering (DLS), Fourier-transform infrared (FTIR) spectroscopy, Bicinchoninic acid (BCA) assay, SDS-PAGE, and total phenolic and flavonoid content analyses. The isolated CELEVs showed mean particle size of 99.76 nm while the zeta potential was -20.8 mV. HR-TEM confirmed that the vesicles were spherical-shaped with a diameter below 100 nm. Biochemical characterization revealed that protein enriched vesicles with 2.48 ± 0.06 $\mu\text{g}/\mu\text{L}$ of protein and SDS-PAGE visualized protein bands ranging from 10 to 250 kDa. FTIR analysis demonstrated the presence of functional groups of a protein, lipid and phosphate. Besides, the CELEVs were found to possess a considerable amount of phenolic compounds (0.243 ± 0.037 mg GAE/g) and flavonoids (0.354 ± 0.113 mg QE/g). CELEVs showed good stability during 4 weeks of storage with minimal changes in particle size and zeta potential when stored at Room temperature, 4°C , -20°C , and -80°C . To the best of our knowledge, this is the first systematic report of CELEVs, demonstrating their stability and potential as nanoplatfoms for applications in nanotechnology and biomedicine.

Keywords: *Colocasia esculenta*, Plant-derived extracellular vesicles, Physicochemical characterization, Nanotechnology

Two-Dimensional Nanomaterials for Photocatalytic Antibiotic Degradation in Wastewater: A Comprehensive Review of Material Design, Heterojunction Engineering and Mechanistic Insights

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Abstract

Antibiotic residues in wastewater are an increasing environmental concern because many compounds persist and are not completely removed by conventional treatment methods. Photocatalysis has emerged as a promising approach for degrading pharmaceutical contaminants under light irradiation. This review examines two-dimensional (2D) nanomaterials, including graphene/GO/rGO, g-C₃N₄, MXenes, MoS₂, WS₂, LDHs, h-BN, COFs, and 2D heterojunctions, with emphasis on material design, characterization, photocatalytic mechanisms, and wastewater treatment. Structural and morphological properties are investigated through XRD, Raman spectroscopy, FESEM, TEM/HRTEM, SAED, and AFM, while XPS, FTIR, EDS, and BET provide information on surface chemistry, bonding, elemental composition, and surface properties. Optical and electronic properties are evaluated using UV–Vis DRS, PL, EIS, photocurrent response, and Mott–Schottky analysis. Advanced techniques such as EPR and LC-MS help identify reactive oxygen species and degradation intermediates. The reviewed literature indicates that suitable 2D heterojunctions can improve charge separation and promote reactive species such as $\cdot\text{O}_2^-$ and $\cdot\text{OH}$, enhancing antibiotic degradation. Catalyst stability, recyclability, mineralization, and real wastewater performance are also considered. Overall, integrated characterization linking structure, interfaces, electronic properties, ROS generation, and degradation pathways is essential for developing efficient and sustainable 2D photocatalysts for antibiotic-contaminated wastewater treatment. Overall, this review highlights their potential for sustainable wastewater treatment.

Keywords: 2D nanomaterials, Photocatalysis, Antibiotic degradation, Heterojunction engineering

Sustainable Nanocomposite Membrane Based on Areca Palm Plate-Derived CMC for Adsorption and Photocatalytic Water Treatment

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Abstract

This paper is focused on improving the adsorption behavior for application in water purification and in photo catalytic efficiency of activated carbon (AC) and nano TiO₂ by formulating new composite membrane with CarboxylMethyl Cellulose (CMC), Chitosan (Ch) and Polyvinyl Pyrrolidone (PVP). CMC is prepared from waste material, Areca Palm Plates. Cellulose is prepared by alkali, bleaching, and acid hydrolysis treatment, and its derivative carboxymethyl cellulose is obtained through alkalization followed by etherification Sol-gel Method is employed to prepare nano TiO₂ Particles. The crystallite size of the nano-TiO₂ particles was found to be around 64nm which was calculated by Bragg's equation. Water Purification test is analyzed using UV-Visible Spectrophotometer. The nanocomposite thin film membrane achieved 61% purification of sludge water. Rhodamine B dye, commonly used in textile industries, is selected for photodegradation studies. The nanocomposite exhibits a high degradation of 81% after 2 hours of time period on rhodamine B dye solution. Soil degradation test showed that the prepared composite film showed 86% of weight loss after 16 days. Antibacterial studies were examined using *Staphylococcus aureus* and *Escherichia Coli* using Ampicillin as standard. This study, therefore, focuses on a nanocomposite thin film that not only acts as an efficient adsorbent for water purification but also shows excellent capability in degrading Rhodamine B dye under photodegradation conditions.

Keywords: Areca Palm Plates, Carboxy Methylcellulose, Activated Charcoal, Rhodamine B dye, Nanocomposite thin film membrane.

**Studies on the Structural, Nonlinear Optical,
Antimicrobial Activity of Tert-Butylamine Methyl-Ptoluene Sulphonate
Single Crystal**

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Abstract

Tert-butylamine methyl-P-toluene sulphonate (BAMTS), an organic single crystal, was grown at room temperature using the slow evaporation method. SXRD investigations reveal that BAMTS belong to the monoclinic system and space group $C 2/c$ with Z 8. The functional groups are found using FTIR analysis. UV-Vis spectroscopy, which includes optical absorption, is used to calculate the band gap energy and optical characteristics. The cut-off wavelength is identified as a 254 nm. The Band gap energy is found to be 3.0209 eV. BAMTS' SHG efficiency is 1.8 times than that of standard KDP. Fluorescence investigations were used to assess the luminous effect. The antibacterial and antifungal activities of formed crystals are more effective against species/than references.

Keywords: organic single crystal, monoclinic system, lattice parameters, optical absorption, luminous effect, SHG efficiency.

Synthesis and Characterization of Enzyme Based Systems for Microplastic Degradation

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Abstract

Microplastics are persistent environmental contaminants that accumulate in aquatic ecosystems and enter food chains, posing potential risks to living organisms. Their diverse polymeric composition, including polyethylene terephthalate (PET), polypropylene (PP), and high-density polyethylene (HDPE), makes their removal and degradation challenging. This study investigated fungal derived extracellular enzymes for microplastic biodegradation and evaluated an immobilized lipase system for plastic degradation. Water samples collected from different locations in Coimbatore were filtered and analyzed for microplastics, which were characterized based on morphology and polymeric properties. Fungal isolates were obtained and screened for their ability to grow in microplastic containing media and utilize polymers as potential substrates. Microplastic degradation was assessed using UV-Visible spectroscopy, scanning electron microscopy (SEM), and weight-loss measurements. Lipase was subsequently immobilized and applied to plastic substrates to evaluate degradation efficiency and retained enzymatic activity. Molecular docking studies were performed using AutoDock to investigate enzyme-substrate interactions, and BIOVIA was used for two dimensional and three-dimensional visualization of the complexes. Microplastics were detected in the analyzed water samples, and fungal isolates demonstrated degradation potential. Treated samples exhibited changes in UV-Vis absorbance, polymer surface morphology, and mass, indicating degradation associated alterations. Immobilized lipase treatment resulted in measurable weight loss while retaining enzymatic activity. Docking analysis demonstrated favorable enzyme-substrate interactions, supporting the potential of enzyme-mediated plastic degradation. Overall, the findings highlight fungal derived enzymes and immobilized lipase as promising biological approaches for sustainable microplastic degradation and mitigation of plastic pollution in aquatic environments.

Keywords: Microplastics, Microorganisms, Immobilized Enzymes, Molecular docking, Sustainability

PP-ESC - 01

A Comprehensive Study of Functionalized Graphene Oxide with Enhanced Epoxy Coatings for Superior Corrosion Resistance and Adhesion

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Abstract

Corrosion of mild steel remains a critical challenge across construction, automotive, and marine industries, leading to substantial structural degradation and economic losses. Conventional epoxy coatings, though widely used as protective barriers, often lose efficacy due to microscopic defects that permit corrosive agent penetration. This study addresses this limitation by synthesizing functionalized graphene oxide (f-GO) via a modified Hummer's method and incorporating it into epoxy coating matrices applied to mild steel substrates, with green pigments and environmentally friendly plant- and amino-acid-derived inhibitors adsorbed onto the GO surface to enhance sustainability. The functionalized coatings were comprehensively characterized using Gas Chromatography-Mass Spectrometry (GC-MS), Fourier Transform Infrared (FTIR) spectroscopy, UV-Visible spectroscopy, and Field Emission Scanning Electron Microscopy (FE-SEM), alongside adhesion tape testing (ASTM D3359-23), salt spray testing (ASTM B117-16), and contact angle measurements on steel and aluminum surfaces. GC-MS identified 64 bioactive compounds, including phytol and octadecatrienoic acid, contributing corrosion-inhibiting potential, while FTIR confirmed characteristic functional groups such as hydroxyl, carbonyl, and aromatic moieties. FE-SEM revealed a uniform, defect-free coating microstructure, and contact angle analysis demonstrated enhanced hydrophobicity (up to 72.4° on steel). The f-GO/epoxy coatings withstood over 300 hours of salt spray exposure without rust formation and exhibited excellent adhesion with no peeling during tape testing. These findings confirm that f-GO significantly improves the barrier properties, adhesion strength, and overall corrosion resistance of epoxy coatings, presenting a promising, eco-friendly advancement in protective coating technology for industrial applications.

Keywords: *Functionalized graphene oxide; Epoxy coatings; Corrosion resistance; Adhesion strength; Green inhibitors; Mild steel; Surface hydrophobicity*

Integrating Machine Learning with Eco-Friendly Analytical Platforms for Enhanced Performance

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Abstract

Green analytical techniques have received a global attention in recent decades, especially in researchers and play a key role in pharmaceutical industry and laboratories. It reduce the toxic environmental impact by minimizing the hazardous substances, energy consumption, re-use of energy sources, and improves availability of the precise, sensitive and, reliability of the analytical tools. In the growing research activity on sustainable, environmental friendly and reduce toxicity are more significant area. Traditional analytical tools are very costly and consume large volume of organic solvents. In this regards, green analytical chemistry has more focusing on reducing hazardous substances, minimize the waste, increase energy effectiveness, and advanced eco-friendly tools. Recent evolution in Hyphenated techniques, play a vital role in the green analysis of the samples for separation, identification, and quantification, which includes GC-MS, LC-MS, LC-NMR, CE-MS. Greenness tools gained more prominence and environmental friendly substances approach such as NEMI, GAPI, AGREE, AGREE prep for assessment procedure. These systems provide high sensitivity, selectivity, and reproducibility, making them indispensable in fields such as pharmaceuticals, environmental monitoring, food safety, and metabolomics. This review aims to provide a comprehensive overview of recent developments in AI-assisted green method development within hyphenated analytical techniques. It highlights key technologies, applications, advantages, and limitations, while also discussing future perspectives for achieving more sustainable and intelligent analytical systems. It is important to develop and innovate new analytical tools with minimized toxic impact on environment.

KEYWORDS: Hyphenated techniques, GC-MS, LC-MS, NEMI, GAPI, AGREE, Green analytical chemistry (GAC)

Facile Citrus Plant-Part Mediated Fabrication Of Co-Precipitated, Surface-Engineered Green-Synthesis Of ZnO Material For Effective Photocatalytic Degradation of Selective cationic And Anionic Dyes and Post-Photocatalytic Antioxidant Capacity

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Abstract

Water pollution caused by dye-contaminated industrial wastewater has now become a major environmental concern, as persistent and chemically stable synthetic dyes can adversely affect aquatic ecosystem as well as human health. Conventional treatment approaches have shown limited effectiveness, while adsorption can generate secondary solid waste. Photocatalytic dye-degradation provides a more sustainable alternative by transforming dye molecules into smaller degradation products. This study reports the plant-part-mediated green synthesis of ZnO material using Citrus medica leaf and fruit peel extracts and investigates their distinct surface properties and dye-selective photocatalytic degradation of cationic and anionic dyes under natural sunlight irradiation. The resulting material, ZNP_LEAF and ZNP_PEEL, exhibited distinct physiochemical and surface characteristics, with ZNP_LEAF showing a strongly negative surface charge (-45.97 mV), while ZNP_PEEL exhibited higher surface area (443618 m²g⁻¹) and slightly positive surface charge (+3.36 mV). ZNP_LEAF preferentially degraded the cationic dye- Methylene blue (MB), showing approximately 4.51 times higher initial degradation rate than ZNP_PEEL, whereas ZNP_PEEL showed approximately 3.64 times higher initial degradation rate towards the anionic-dye Methyl orange (MO). Higher significant BBD RSM models ($R^2 = 0.9893$ and 0.9895) were used to optimize the material-dye systems, indicating that most significant role is played by the reaction mixture pH and to achieve 97.08% MB and 97.74% MO dye degradation. ROS studies demonstrated superoxide radical and hydroxyl radical as dominant for ZNP_LEAF-MB and ZNP_PEEL-MO systems. Both materials retained photocatalytic activity after five cycles and measurable antioxidant activity post-treatment. Overall, plant-part selection effectively tuned ZnO surface properties and dye-selective photocatalytic performance, demonstrating its potential for sustainable waste-water remediation.

Keywords: Citrus medica; ZnO material; Methylene Blue; Methyl Orange; Photocatalytic dye degradation.

Chemically extracted Fish Scale type I collagen is modified using Ultrasound-Mediated Post-extraction Treatment, both Structurally and Function

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Abstract

Fish scales are a valuable source of type I collagen that can be used in biomaterials. In the present study, type I collagen was extracted chemically from fish scales and later treated with controlled ultrasound treatment for the post-extraction process to explore the process of structural and morphological remodeling induced by ultrasound. Since the approaches of ultrasound-assisted extraction cannot remove the structural effect of ultrasound, the present study adopted the approach of ultrasonic separation after collagen isolation, which enabled the study of the structural effect of ultrasound without shaking the extraction system. The scaling was carried out under alkaline condition followed by demineralization and extraction with 0.5 M acetic acid and processed fish scales. Processed fish scales were subjected to alkaline treatment and then demineralization was carried out followed by extraction with 0.5 M acetic acid. The collagen extracted was then subjected to ultrasound treatment at 25 kHz at 70% power for 10 min with controlled temperature conditions and the untreated chemically extracted collagen was used as control. FTIR and SEM were used to evaluate their structural and morphological changes. FTIR analysis detected significant shifts in the characteristic collagen amide regions post ultrasound treatment (amide A band from 3071 to 3432 cm⁻¹, amide I band from 1654 to 1611 cm⁻¹); suggesting changes in the hydrogen-bonding environment and/or molecular organization of collagen. SEM analysis revealed significant changes in the fibrillar architecture, showing a mean fibre diameter from 6.29 µm to 2.93 µm, or a 53.4% decrease. These results taken together indicate that controlled post-extraction ultrasound causes measurable molecular and fibrillar remodeling of the fish scale-derived Type I collagen, and suggest acoustic cavitation as a method to control the remodeling of extracted collagen.

Keywords: Fish scale collagen; Type I collagen; Post-extraction ultrasound; Acoustic cavitation; FTIR; SEM; Structural remodeling; Fibrillar architecture.

Impact of Ultrasound on Microbial Reduction of Coconut Sap (Neera)

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Abstract

Coconut inflorescence sap (Neera) is a nutritious beverage that is enriched with sugars and minerals; yet it is highly perishable due to its susceptibility to rapid fermentation through the action of a heterogeneous microbial population. The present study focused on the use of ultrasound as a non-thermal processing technique to reduce the rate of microbial proliferation and delay fermentation of coconut Neera. Fresh Neera samples procured from the coconut-growing regions of Tamil Nadu, India, were processed using probe-type high-intensity ultrasound at 20 kHz and amplitudes of 30%, 47%, and 99% for 2.2, 4.7, and 10 min, respectively. The ultrasound-processed and unprocessed control samples were stored at 4 ± 1 °C and analyzed at 6-h intervals for up to 36 h for microbial enumeration. The population of total viable bacteria, lactic acid bacteria, and yeast was monitored to evaluate the effect of treatment on microbial proliferation and fermentation. Overall, the highest reduction in microbial load and delayed microbial proliferation was achieved for 99% ultrasound amplitude for 10 min treatment. The results demonstrated that high-intensity ultrasound reduced the initial microbial load and inhibited the subsequent proliferation of microorganisms, allowing the treated Neera sample to be stored for a longer period (36 h) than control sample. The heterogeneity of the microbial population and potential enzymatic activity are responsible for shelf-life extension. Further studies on enzyme activity and inactivation, along with individual and combined preservation strategies, are required to extend shelf-life of coconut Neera.

Keywords: Coconut Neera, *Cocos nucifera* L., High-intensity ultrasound, Microbial reduction, Microbial proliferation, Fermentation control, Shelf-life extension, Microbial enzymes.

Does Bora/Aza Substitution Affect the ERO of Benzofused Oxetenes – A Density Functional Insight

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Abstract

Aromaticity enhancement and aromaticity depreciation are known to affect the pericyclic reactions. The rapid Electrocyclic ring closure (ERC) of orthoquinodimethane to form benzocyclobutene is due to the gain in the aromaticity in fused benzene ring and the reverse is less facile owing to similar reasons. The effect of boron and nitrogen substitution in the ring fused with oxetene on the Electrocyclic ring opening (ERO) of benzofusedoxetenes have been studied at B3LYP 6-31G(d) level. Thermodynamic and kinetic parameters have been computed. NICS, FMO and NBO analysis have been performed to throw light on the role of aromaticity in these reactions. Indeed the hetero atoms on the fused ring have affected the ERO of oxetene. Effect of boron substitution gives an exalted NICS(0) value which has been interestingly explained by the negative hyperconjugation.

Formulation and evaluation of Herbal ointment from *Azadirachta indica* and *Ocimum Tenuiflorum* Leaf

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Abstract

The present study focuses on the formulation and evaluation of an herbal ointment prepared from the methanolic leaf extracts of *Azadirachta indica* (Neem) and *Ocimum tenuiflorum* (Tulsi). The leaves were collected, shade-dried, powdered, and extracted using methanol. Preliminary phytochemical screening indicated the presence of important constituents such as alkaloids, glycosides, terpenoids, flavonoids, tannins, saponins, and steroids in the extracts. Thin-layer chromatography was performed for preliminary characterization of the extracts. The herbal ointment was formulated using stearic acid, yellow beeswax, triethanolamine, propylene glycol, herbal extracts, and rose oil. The prepared formulation was evaluated for colour, odour, consistency, pH, spreadability, loss on drying, solubility, washability, and non-irritancy. The formulation showed a light-green colour, smooth consistency, pH 5.7, good washability, and was reported to be non-irritant. The study indicates that the combined extracts of Neem and Tulsi can be incorporated into a topical herbal ointment and may provide a useful plant-based formulation for skin-related applications. Further phytochemical and pharmacological studies are required to establish its effectiveness.

Keywords: *Azadirachta indica*; *Ocimum tenuiflorum*; Neem; Tulsi; Herbal ointment; Methanolic extract; Phytochemical screening; TLC; Topical formulation; Antifungal activity.

Green Nanotechnology Meets Wound Healing: *Cissus Quadrangularis*-Mediated Silver Nanoparticles for Diabetic Foot Ulcer Therapy

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Abstract

Diabetic foot ulcer (DFU) is a serious complication of diabetes mellitus, characterized by delayed wound healing, persistent inflammation, oxidative stress, and increased susceptibility to microbial infection. Conventional wound-management approaches may have limitations in promoting effective tissue regeneration while controlling infection and oxidative damage. The present study focuses on the green synthesis of silver nanoparticles (AgNPs) using *Cissus quadrangularis* extract and their potential application in the management of diabetic foot ulcers. *Cissus quadrangularis*, a medicinal plant traditionally recognized for its wound-healing, antioxidant, and anti-inflammatory properties, was selected as a natural reducing and stabilizing agent for nanoparticle synthesis. The synthesized AgNPs were characterized using suitable analytical techniques, including UV–Visible spectroscopy, Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), dynamic light scattering (DLS), and zeta potential analysis. The antioxidant potential of the plant extract and synthesized nanoparticles was evaluated using the DPPH radical-scavenging assay. In addition, the antimicrobial activity of the synthesized AgNPs was investigated against selected pathogenic microorganisms associated with wound infections. The green synthesis approach provides an eco-friendly and cost-effective alternative to conventional nanoparticle synthesis by minimizing the use of hazardous chemicals. The incorporation of phytoconstituents from *Cissus quadrangularis* may provide synergistic antioxidant, antimicrobial, and wound-healing benefits. Overall, the study highlights the potential of *Cissus quadrangularis*-mediated AgNPs as a promising phyto-genic nanomaterial for future development of advanced therapeutic approaches for diabetic foot ulcer management.

Keywords: *Cissus quadrangularis*, silver nanoparticles, green synthesis, Diabetic foot ulcer, Wound healing, Nanotechnology.

Development and Characterization of a Bassorin-Based Hydrogel Incorporating *Clerodendrum inerme* Leaf Extract for Anti-bacterial and Anti-Biofilm Applications

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Abstract

The increasing prevalence of antibiotic-resistant microorganisms and biofilm-associated infections has created a need for safe, effective, and sustainable alternatives for wound management. Hydrogels are promising biomaterials for wound care owing to their high waterholding capacity, biocompatibility, and potential to provide a suitable environment for controlled therapeutic delivery. The present study focuses on the development and characterization of a Bassorin-based hydrogel incorporating *Clerodendrum inerme* leaf extract for antibacterial and anti-biofilm applications. Initially, *Clerodendrum inerme* leaves were subjected to extraction and qualitative phytochemical screening. The preliminary analysis indicated the presence of phenolic compounds, flavonoids, saponins, alkaloids, and glycosides, suggesting the presence of biologically active constituents. Quantitative estimation of total phenolic content (TPC) is currently in progress, while further evaluation of total flavonoid content (TFC) and antioxidant activity using ABTS and FRAP assays is planned. The Bassorin fraction will be isolated from Gum Tragacanth and incorporated with the leaf extract to formulate and optimize the hydrogel. The formulated hydrogel will be characterized for pH, viscosity, spreadability, swelling index, in vitro release, stability, FTIR, and SEM analysis. The developed formulation is expected to demonstrate favorable physicochemical properties, swelling behavior, controlled release characteristics, antioxidant activity, antibacterial activity, and anti-biofilm potential. Therefore, the proposed Bassorin-based hydrogel incorporating *Clerodendrum inerme* leaf extract may serve as a promising natural biomaterial for wound-care and biomedical applications, subject to further experimental validation.

Keywords: *Clerodendrum inerme*, Bassorin-based hydrogel, antibacterial, anti-biofilm

Univariate Harmonization Does Not Guarantee Removal of Multivariate Site Information in Multi-Centre Prostate MRI Radiomics

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Abstract

Quantitative image biomarkers (radiomics) extracted from MRI are highly sensitive to scanner and acquisition-protocol differences, which is a primary barrier to multi-centre reproducibility of imaging-based biomedical models. ComBat harmonization is the field's default correction, yet its success is almost always certified by per-feature statistics alone. We asked whether removing site association feature by feature actually removes site information from the feature set. We analysed 115 T2-weighted prostate MRI examinations with expert whole-gland segmentation from six public clinical sites, and externally validated on 278 examinations from two independent PI-CAI centres and 139 Prostate158 cases. After isotropic resampling, 107 PyRadiomics features were extracted. Site effects were quantified by Kruskal–Wallis testing (Benjamini–Hochberg and Bonferroni correction), PCA, and a Random Forest site classifier under 5-fold stratified cross-validation, before and after correction. Four strategies were compared — parametric ComBat, non-parametric ComBat, CovBat, and a naive per-site z-score baseline — and the correction was audited with SHAP attribution, SHAP interactions, accumulated local effects, LIME, and a counterfactual analysis comparing the classifier's own de-identification direction with ComBat's actual correction. Before harmonization, 106/107 features differed significantly by site and a Random Forest recovered the acquisition site with 87.8% accuracy (chance 16.7%). Per-feature correction was highly effective: ComBat left 4/107 site-associated features, CovBat 2/107, and the z-score baseline none. Multivariate site information nevertheless persisted. Under the conventional protocol, in which the correction is estimated once on the complete dataset, site-classifier accuracy fell from 0.878 to 0.765; when ComBat was instead estimated on the training fold and applied to held-out data, accuracy returned to 0.878, showing that the apparent reduction was largely an artefact of estimating the correction on data containing the evaluation folds. Externally, the per-feature reduction replicated (91/107 to 14/107) while site accuracy remained at or above its raw-feature value of 0.907. In both cohorts the residual signature was recovered by tree-ensemble classifiers and not by linear ones, locating it in non-linear multivariate structure rather than a residual location–scale offset. Anatomical fidelity was preserved (gland-volume Spearman $\rho = 0.908$ internally; $\rho = 0.903$ against clinically measured volume externally). Per-feature statistical decontamination is insufficient to certify successful radiomic harmonization. Certification should additionally examine multivariate site identifiability estimated without evaluation-fold information, biological fidelity against a reference independent of the segmentation mask, feature-space geometry, and leakage-free downstream performance. All code, feature tables and the pre-specified analysis protocol are released for reproduction.

Keywords: radiomics; multi-centre MRI; ComBat harmonization; batch effects; reproducibility; explainable AI

Synthesis and Characterization of Liposomal Encapsulated Particles for Enhanced Therapeutic Efficiency in L929 Cell Lines

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Abstract

Medicinal plants are important sources of bioactive compounds with potential applications in the prevention and management of various diseases. *Gymnema sylvestre*, commonly known as “Gurmar” or the “sugar destroyer,” is a woody climbing plant traditionally used in Indian medicine for its antidiabetic properties, particularly its ability to help regulate blood glucose levels and suppress the perception of sweet taste. Gymnemic acid, a major bioactive constituent of *G. sylvestre*, has demonstrated promising therapeutic potential; however, its effective delivery may be limited by its physicochemical and bioavailability characteristics. The present study aims to develop a lipid-based carrier system for the encapsulation and delivery of gymnemic acid to enhance its therapeutic efficacy and improve its delivery characteristics. Gymnemic acid will be incorporated into the lipid-based carrier, and the developed formulation will be evaluated for its physicochemical properties and drug-loading efficiency. Qualitative and quantitative estimation of gymnemic acid will be performed using suitable analytical methods, including UV–Visible spectrophotometry. The optimized formulation will be characterized using Fourier-transform infrared spectroscopy (FTIR), particle size, polydispersity index (PDI), and zeta potential measurements to investigate drug–carrier interactions, functional groups, particle-size distribution, surface charge, and formulation stability. Furthermore, the optimized formulation will be evaluated *in vitro* using the L929 cell line to determine its cellular compatibility and preliminary therapeutic potential. Overall, the study is expected to provide a promising lipid-based delivery approach for gymnemic acid and may contribute to the development of a safer, efficient, and more targeted system for its therapeutic application.

Keywords: Gymnemic acid, Lipid based carrier, Encapsulation, Therapeutic efficiency.

Extraction of Oil from Lemongrass and its Application in Cosmetic Product Development

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Abstract

The present study focused on the extraction, characterization, and cosmetic application of essential oil derived from *Cymbopogon citratus* (lemongrass). Fresh leaves were collected, authenticated, and subjected to steam distillation to obtain citral-rich essential oil. The oil was characterized using FTIR, GC–MS, and physicochemical analysis, confirming the presence of aldehydes, terpenes, and phenolic compounds. Antimicrobial activity was evaluated against *Staphylococcus aureus*, *Escherichia coli*, *Salmonella typhi*, and *Candida albicans*, demonstrating strong inhibition in a dose-dependent manner. Antioxidant assays highlighted the potential of lemongrass oil as a natural preservative and therapeutic agent. The oil was incorporated into herbal soap and shampoo formulations, which were further assessed for physicochemical and functional properties. Results revealed that the soap exhibited high total fatty matter (68%), stable foaming capacity, and antimicrobial efficacy, while the shampoo showed a scalp-friendly pH (6.3), excellent foaming ability, suitable viscosity, and antimicrobial activity against *Staphylococcus aureus* and *Corynebacterium diphtheriae*. Sensory evaluation confirmed favorable consumer attributes, including smooth lather, refreshing aroma, and enhanced softness and shine of hair. Overall, the findings validate lemongrass oil as a multifunctional bioactive ingredient suitable for natural cosmetic formulations, supporting its role in sustainable and eco-friendly personal care products.

Keywords: Lemon grass and oil; Soxhlet extraction; GC–MS; FTIR; Antibacterial activity; Cosmetic formulations; Natural antioxidant

Isolation, Characterization, and Antirepellent Potential of Eugenol and Asarone from *Syzygium aromaticum* and *Acorus calamus*

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Abstract

Mosquito-borne diseases such as malaria, dengue, chikungunya, yellow fever, and Zika continue to be major global public health concerns, with *Aedes aegypti* acting as a primary vector. Increasing environmental and health concerns regarding synthetic repellents such as DEET have led to growing interest in plant-based eco-friendly alternatives. Natural compounds such as eugenol from *Syzygium aromaticum* (clove) and asarone from *Acorus calamus* (vasambu) have demonstrated promising insect repellent and insecticidal properties. The present study focuses on the biosynthesis of zinc oxide nanoparticles (ZnONPs) using flower bud extracts of *Syzygium aromaticum* and root extracts of *Acorus calamus*, along with the evaluation of their phytochemical constituents, antibacterial activity, and potential antirepellent properties. ZnONPs were synthesized at room temperature using 2 mM zinc sulphate through the boiled extract method. The synthesized SaZnONPs and AcZnONPs were characterized using UV–Visible spectroscopy, FTIR, SEM, and EDX analysis. The UV–Vis spectrum showed an absorption peak at 365 nm, while SEM analysis confirmed nanoparticle sizes ranging from 30–90 nm. FTIR analysis indicated the presence of organic functional groups responsible for nanoparticle stabilization. Phytochemical screening of methanolic and chloroform extracts revealed the presence of glucose, proteins, phenols, flavonoids, terpenes, and saponins, confirming the presence of biologically active compounds. The antibacterial activity of the synthesized nanoparticles was evaluated using the well diffusion method against both Gram-positive (*Staphylococcus* sp., *Enterococcus* sp.) and Gram-negative (*Escherichia coli*, *Klebsiella* sp.) bacteria, demonstrating significant inhibitory effects. The findings suggest that ZnONPs synthesized from *Syzygium aromaticum* and *Acorus calamus* possess considerable bioactive potential and may serve as eco-friendly alternatives for developing effective commercial antirepellent products in the future.

Keywords: Zinc oxide nanoparticles, *Syzygium aromaticum*, *Acorus calamus*, Phytochemical analysis, Antibacterial activity.

Sustainable Valorization of Biowaste through Organic-Polymeric Hybridization of Hydroxyapatite for Diverse Biomedical Applications

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Abstract

The valorization of biowaste into functional biomaterials offers a sustainable strategy for addressing both environmental and biomedical challenges. In this study, caprine femur bone-derived hydroxyapatite (HAP) was transformed into an organic–polymeric hybrid composite through incorporation of 5-amino 4-imidazolecarboxamide (AICA), sodium alginate (SA) and polyacrylonitrile (PAN), generating the m-HAP-3 system. The resulting material was investigated to determine whether organic–polymeric hybridization could extend the functional utility of biogenic HAP across distinct biomedical contexts. As a titanium surface-engineering material, m-HAP-3 exhibited improved coating integrity, interfacial adhesion, mechanical performance, corrosion resistance and antibacterial functionality compared with HAP. In parallel, the biological responses of HAP and m-HAP-3 were evaluated using MDA-MB-231 and NIH3T3 cells. Both materials produced comparable concentration-dependent effects on MDA-MB-231 viability, accompanied by ROS generation, mitochondrial-associated alterations and cellular/nuclear morphological changes, while maintaining comparatively high viability in NIH3T3 cells under the investigated conditions. Collectively, the findings demonstrate that organic–polymeric hybridization enhances the functional performance of biogenic HAP particularly at the titanium–coating interface, while retaining its inherent cellular response. Thus, a single sustainably derived HAP-based hybrid platform can provide diverse and application-specific biomedical functionality, establishing a promising foundation for further biomaterial and biological investigations.

Keywords: Biowaste valorization; Biogenic HAP; Organic-polymeric hybrid; Surface activated Ti coating; Electrophoretic deposition; Triple-negative breast cancer

Eco-Friendly Phytochemical-Assisted Synthesis of Zinc Oxide Nanoparticles from *Nilgirianthus Ciliates* and *Urochola Ramose* with Antioxidant and Anticancer Evaluation

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Abstract

This study focuses on the eco-friendly synthesis of zinc oxide nanoparticles (ZnO NPs) using phytochemical-rich extracts of *Nilgirianthus ciliatus* and *Urochloa ramosa*. The synthesized ZnONPs will be characterized for their size, morphology, crystalline structure, functional groups, and optical properties. Their antioxidant and anticancer activities will be evaluated using suitable in vitro assays. A comparative analysis will determine the relative biological efficacy of nanoparticles synthesized from both plant sources, highlighting their potential for sustainable nanomedicine and pharmaceutical applications.

Keywords: Zinc oxide nanoparticles, *Nilgirianthus ciliatus*, *Urochloa ramosa* Antioxidant activity, Anticancer activity.

Comprehensive Chemical Characterization and Bioactivity Analysis of *Myristica malabarica* Seed Extract

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Abstract

The study explores the phytochemical profile and bioactivity of the ethanolic seed extract of *Myristica malabarica*, a traditionally used medicinal species. Seeds collected from the Kolli Hills, Tamil Nadu, were subjected to ethanolic extraction and were analyzed by LC–MS, GC–MS, FTIR and ¹H NMR. LC–MS identified malabaricone A (m/z 327.05) as the major constituent, while GC–MS revealed α -cardanolide and β -coprostane triterpenoids. FTIR and NMR confirmed the presence of phenolic, carbonyl and alkene functional groups characteristic of diarylnonanoids. The extract showed potent DPPH radical scavenging activity ($IC_{50} = 21.05 \mu\text{g/mL}$) and significant α -amylase inhibition ($IC_{50} = 40.8 \mu\text{g/mL}$), correlating with its phenolic and flavonoid content. These findings confirm the antioxidant and antidiabetic potential of *M. malabarica* and support its ethnomedicinal relevance. The seed extract represents a promising natural source for developing plant-based therapeutic formulations.

Keywords: *Myristica malabarica*, Malabaricone A, Antioxidant, α -Amylase inhibition, Phytochemistry.

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

Green Synthesis of Silver Nanoparticles Using *Nilgiranthus Ciliatus* and *Urochloa Ramosa* and their Antioxidant and Anticancer Activities

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Abstract

The present study focuses on the green synthesis of silver nanoparticles (AgNPs) using phytochemical-rich extracts of *Nilgiranthus ciliatus* and *Urochloa ramosa* as natural reducing and stabilizing agents. This eco-friendly approach provides a sustainable alternative to conventional nanoparticle synthesis by reducing the use of hazardous chemicals. The synthesized AgNPs will be characterized using appropriate analytical techniques to determine their particle size, morphology, crystalline structure, surface functional groups, and optical properties. The role of plant-derived phytochemicals in the reduction and stabilization of AgNPs will also be investigated. Furthermore, the synthesized nanoparticles will be evaluated for their in vitro antioxidant and anticancer activities using suitable biological assays. A comparative assessment of AgNPs synthesized from both plant extracts will be performed to determine their relative biological efficacy. The study is expected to demonstrate the potential of *N. ciliatus* and *U. ramosa* as sustainable sources for the synthesis of biologically active silver nanoparticles with potential applications in nanomedicine and pharmaceutical research.

Keywords: Silver nanoparticles, *Nilgiranthus ciliatus*, *Urochloa ramosa*, Antioxidant activity, Anticancer activity

Green Synthesis of Iron-Copper Bimetallic Nanoparticles from *Brassica Oleracea* and Evaluating their Anticancer and Antidiabetic Activities

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Abstract

Cervical cancer and type 2 diabetes mellitus represent two major interconnected global health challenges driven by oxidative stress (OS) and metabolic dysregulation. This study reports the green synthesis of Fe-Cu bimetallic nanoparticles (BF-FCNPs) using the aqueous extract of *Brassica oleracea* flower (BF-AE) as both reducing and capping agent. The extract was standardised through phytochemical quantification. The synthesized BF-FCNPs were characterized and their antioxidant potential evaluated using ABTS and FRAP. In vitro porcine pancreatic α -amylase (PPAA), a key target for post prandial glucose management. Additionally, the anticancer efficacy of the BF-FCNPs was assessed against HeLa cells. BF-AE was rich in phenols, flavonoids, tannins, and alkaloids (TPC = 0.56 ± 0.07 mg GAE/g; TFC = 0.18 ± 0.02 mg RE/g). BF-FCNPs synthesis was confirmed by color change from colorless to brown, a characteristic UV-Vis SPR broadened peaks at 265, 335 nm; amorphous XRD pattern, quasi-spherical morphology with aggregation, elemental composition showed presence of Fe, Cu, C, and O atoms. FTIR peaks indicating polyphenol capping. BF-FCNPs displayed moderate ABTS radical scavenging ($IC_{50} = 403.38$ μ g/mL) and strong ferric-reducing activity at 20–100 μ g/mL. BF-FCNPs inhibited PPAA in a dose-dependent, non-competitive manner with $K_i = 288.9$ μ g/mL. In HeLa cells, BF-FCNPs caused concentration-dependent cytotoxicity (12.5–200 μ g/mL), morphological disruption, elevated intracellular ROS formation, and progression of apoptosis from early to late stages. This study provides a foundation for further development of BF-FCNPs as biocompatible agents for managing comorbid conditions involving OS and dysregulated carbohydrate metabolism.

Keywords: Biogenic synthesis, Fe-Cu nanoparticles, porcine pancreatic α -amylase, HeLa cells, anticancer, antioxidant.

Integrated Phytochemical, In Vitro and in Silico Evaluation of Wound Healing Potential of *Croton Bonplandianus*

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Abstract

Wound healing is a complex biological process involving coordinated cellular events, and its impairment is often associated with oxidative stress and prolonged inflammation. Medicinal plants are considered promising alternatives due to their diverse phytochemical composition and multi-targeted biological effects. The present study aimed to evaluate the wound healing potential of the ethanolic extract of *Croton bonplandianus* (CBE) using an integrated *in vitro* and *in silico* approach. Phytochemical screening and quantitative estimation confirmed the presence of phenolics and flavonoids, while GC–MS analysis identified a range of bioactive compounds, including fatty acid esters and phenolic derivatives. Antioxidant activity was assessed using ABTS and FRAP assays, where the extract exhibited concentration-dependent free radical scavenging activity. Anti-inflammatory activity was evaluated using protein denaturation and HRBC membrane stabilization assays, showing measurable inhibitory effects. Cytocompatibility studies using L929 fibroblast cells indicated that the extract was non-toxic across tested concentrations. Wound healing activity assessed through a scratch assay demonstrated enhanced fibroblast migration and accelerated wound closure in treated groups compared to the control. Molecular docking analysis revealed stable interactions of selected phytochemicals with IL-1 β and TGF- β 1. In conclusion, CBE exhibits antioxidant, anti-inflammatory, and wound healing properties, supporting its traditional use and suggesting its potential as a natural therapeutic agent for wound management.

Keywords: *Croton bonplandianus*, wound healing, GC-MS analysis, molecular docking, TGF- β 1

Phytochemical Profiling, TLC Fingerprinting and In Vitro Anticancer Activity of Methanolic Leaf Extract of *Artemisia pallens* (Marikolundhu)

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Abstract

Medicinal plants are an important source of biologically active compounds with potential therapeutic applications. *Artemisia pallens* Wall. Ex DC., commonly known as Marikolundhu, is an aromatic medicinal plant traditionally valued for its pharmacological properties. The present study was undertaken to evaluate the phytochemical constituents, thin-layer chromatography (TLC) fingerprint profile, and in vitro anticancer activity of the methanolic leaf extract of *A. pallens*. Disease-free leaves were collected from Chennai, Tamil Nadu, India, authenticated, shade-dried, powdered, and extracted with methanol by cold maceration. Preliminary phytochemical screening was performed using standard qualitative methods. TLC analysis was carried out using a methanol solvent system, and separated constituents were characterized based on their retention factor (Rf) values. The cytotoxic potential of the extract was evaluated against the HepG2 cell line using the MTT assay. Phytochemical screening revealed the presence of alkaloids, flavonoids, terpenoids, steroids, tannins, and quinones, whereas saponins were not detected. Flavonoids and tannins showed strong positive reactions. TLC analysis revealed three distinct bands with Rf values of 0.63, 0.82, and 0.94. The MTT assay demonstrated concentration-dependent cytotoxicity, with cell viability decreasing from 87.8% at 15.62 µg/mL to 51.5% at 250 µg/mL. The findings suggest that methanolic leaf extract of *A. pallens* contains diverse secondary metabolites and exhibits moderate in vitro anticancer potential. Further investigations involving isolation and characterization of individual bioactive compounds, mechanistic studies, and in vivo evaluation are required to establish its therapeutic significance.

Keywords: *Artemisia pallens*, phytochemical screening, TLC fingerprinting, methanolic extract, HepG2, MTT assay, cytotoxicity.

Phytochemical Profiling and HPLC-Based Characterization of Flavonoids in *Rosa gallica* Hip Extracts with *rbcL* Molecular Authentication

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Abstract

Rosa gallica L. is a medicinally important plant recognized as a source of phenolic and flavonoid compounds. The present study was designed to characterize the phytochemical profile of *R. gallica* hip extracts, quantify flavonoid content, identify major flavonoid constituents by high-performance liquid chromatography (HPLC), and provide molecular authentication using the chloroplast *rbcL* region. Plant material was collected in and around Chennai, Tamil Nadu, India, and authenticated by research officers in pharmacognosy/Siddha research. The plant material was shade-dried, powdered, and extracted using different solvents. Qualitative flavonoid screening was performed by conventional colour reactions, while total flavonoid content was estimated spectrophotometrically using catechin equivalents. For chromatographic profiling, repeated sonication extraction was followed by HPLC-UV analysis using an LC-18 column with an acetonitrile:water (40:60, v/v) mobile phase at 1 mL min⁻¹ and UV detection at 274 nm. The HPLC profile showed rutin (23.6109%) and quercetin (24.2343%) as prominent detected flavonoids, followed by genistein (21.5704%), an unidentified component (12.3966%), biochanin (5.3213%), and additional unidentified peaks. Molecular analysis targeted the *rbcL* region; the source document reports submission of *rbcL* sequences to GenBank under accession numbers JQ867403.1 and OQ557505. Overall, the findings demonstrate that *R. gallica* hip material contains a diverse flavonoid profile and support the combined use of phytochemical, chromatographic, and molecular approaches for botanical characterization.

Keywords: *Rosa gallica*; rose hip; flavonoids; phytochemical screening; HPLC; quercetin; rutin; *rbcL*; molecular authentication

Green Synthesis of Ag-ZnO Nanocomposite using (*Mucuna monoperma*) Leaf Extract and Evaluation of Their *In-Vitro* Antibacterial and Anticancer Activities

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Abstract

In the present study, the green synthesis of silver zinc oxide (Ag-ZnO) nanocomposite using the leaf extract of *Mucuna monoperma* as a natural and eco-friendly reducing and stabilising agent is reported. The plant-mediated synthesis is a simple, cost-effective and environment friendly alternative to the conventional chemical and physical methods for the synthesis of nanoparticles. The physicochemical properties of the synthesised Ag-ZnO nanocomposite will be determined by suitable analytical techniques such as surface morphology, crystalline structure, particle size and functional groups. The synthesised nanocomposite will be evaluated for its biological activities by *in vitro* antibacterial and anticancer assays. Its antibacterial activity will be investigated on selected human pathogenic bacterial strains and its anticancer potential will be evaluated on MCF-7 human breast cancer cell lines by an appropriate cell viability assay. The improved biological activity of Ag-ZnO nanocomposite is attributed to the combined effect of silver and zinc oxide nanoparticles and bioactive phytochemicals in *M. monoperma* leaf extract. The results of this study are expected to reveal the potential of plant-mediated Ag-ZnO nanocomposites as promising materials for biomedical applications.

Keywords: *Mucuna monoperma*, Ag-ZnO, Antibacterial activity, Anticancer activity.

Evaluating the Antioxidant, Antimicrobial and Anticancer Potential: A Comparative Study of Green-Synthesized Silver Nanoparticles and *Elaeocarpus variabilis* Leaf Extract

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Abstract

The present study focuses on the evaluation of antioxidant, antimicrobial and anticancer potential of *Elaeocarpus variabilis* leaf extract and its green synthesised silver nanoparticles (AgNPs). *E. variabilis* is a medicinal plant with a variety of bioactive compounds which may be responsible for its biological activities. The leaf extract will be prepared by a suitable extraction method and will be used as a natural reducing and stabilising agent for the synthesis of silver nanoparticles. The formation and physicochemical properties of the synthesised AgNPs will be confirmed by using UV–Visible spectroscopy, FTIR, XRD, and SEM techniques. The antioxidant activity of leaf extract and AgNPs will be evaluated by suitable in-vitro assays. Antimicrobial activity will be tested against selected bacterial and fungal strains and anticancer potential will be tested by appropriate in-vitro cell-line assay. Biological activities of leaf extract and AgNPs will be comparatively analysed to see if green synthesis improves the potential of plant derived material. This study may provide useful preliminary evidence for the development of plant-based silver nanoparticles with potential pharmaceutical and biomedical applications.

Keywords: Antibacterial activity, Antioxidant activity Anticancer activity, *E. variabilis*.

AI-Driven Metagenomic Profiling for Prediction and Characterization of Antimicrobial Resistance Genes

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Abstract

Antimicrobial resistance (AMR) is a growing global health challenge, driven by the emergence and dissemination of antimicrobial resistance genes (ARGs) across human, animal, and environmental microbial communities. Metagenomic sequencing provides a culture-independent approach for comprehensive characterization of microbial communities and their associated resistome. However, the increasing volume and complexity of metagenomic data require intelligent computational approaches for rapid and accurate identification of resistance-associated genomic signatures. This study proposes an AI-driven metagenomic framework for the prediction and characterization of antimicrobial resistance genes from shotgun metagenomic datasets. The proposed workflow integrates sequence quality assessment, taxonomic profiling, functional annotation, ARG identification, and machine-learning-based prediction. The framework will further investigate the association between ARGs and their microbial hosts, enabling characterization of potential transmission patterns and resistome diversity. AI-based prediction can complement conventional homology-based approaches by identifying previously uncharacterized resistance-associated sequences and prioritizing candidate ARGs for experimental validation. The proposed approach has potential applications in AMR surveillance, environmental microbiome monitoring, infectious disease research, and development of data-driven strategies for antimicrobial resistance management.

Keywords: Metagenomics, antimicrobial resistance, resistance genes, artificial intelligence, machine learning, microbial genomics, AMR surveillance

Phytogetic *Zanthoxylum Asiaticum* Transfersomal Gel: A Novel Approach for Enhanced Cutaneous Delivery and Antioxidant Protection

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Abstract

Oxidative stress is an important factor in the development and progression of dermatological conditions, resulting in cellular damage, inflammation, impaired skin barrier function, and delayed tissue repair. Plant-derived bioactive compounds with antioxidant properties offer a promising approach for topical skin management; however, their effectiveness may be restricted by poor solubility, instability, and limited penetration through the skin. The present study is aimed at developing and evaluating a *Zanthoxylum asiaticum* extract-loaded transfersomal gel for enhanced cutaneous delivery and antioxidant protection. Plant material will be collected, authenticated, shade-dried, powdered, and extracted using an appropriate extraction technique. The extract will be standardized based on extractive yield and preliminary phytochemical screening, followed by evaluation of its antioxidant activity using appropriate in vitro free-radical-scavenging assays. Transfersomes will be prepared using phospholipids and edge activators and optimized by varying critical formulation parameters to obtain stable vesicles with desirable characteristics and high entrapment efficiency. The optimized transfersomes will be characterized for particle size, polydispersity index, zeta potential, morphology, deformability, entrapment efficiency, and physicochemical compatibility. Subsequently, the optimized transfersomes will be incorporated into a suitable topical gel base. The developed transfersomal gel will be evaluated for appearance, homogeneity, pH, viscosity, spreadability, extrudability, extract content, and in vitro release. Ex vivo skin permeation studies will be performed to assess enhanced cutaneous delivery. Biological evaluation will include antioxidant activity and, where feasible, cytocompatibility, intracellular reactive oxygen species reduction, and scratch wound-healing studies. Stability studies will determine formulation stability. The developed formulation is expected to improve skin delivery and antioxidant protection.

Keywords: *Zanthoxylum asiaticum*, transfersomal gel, topical delivery, cutaneous delivery, antioxidant activity, oxidative stress.

Morphological and Morphometric Characterization of Human Lungs with Exploration of Nanotechnology-Based Approaches for Targeted Pulmonary Drug Delivery

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Abstract

Detailed knowledge of pulmonary morphology and morphometry is essential for understanding variations in lung anatomy, planning thoracic procedures, interpreting radiological findings, and optimizing targeted pulmonary therapies. Recent advances in nanotechnology have introduced nanoparticles as potential vehicles for site-specific drug delivery and imaging within the respiratory system. However, the relationship between anatomical variation in lung morphology and the potential distribution of nanoparticle-based therapeutic systems remains inadequately explored. To evaluate the morphological and morphometric characteristics of human lungs and explore their potential implications for nanotechnology-based targeted pulmonary drug delivery. A cross-sectional anatomical study will be conducted using adult human lungs obtained from donated cadavers. Morphological parameters including number and pattern of fissures, lobar configuration, accessory fissures, and external anatomical variations will be documented. Morphometric parameters including lung length, width, thickness, weight, volume, hilar dimensions, and bronchopulmonary segment-related measurements will be recorded. Selected parameters may be correlated with radiological measurements obtained from computed tomography. Based on the anatomical findings, an exploratory nanotechnology component may evaluate the potential suitability of biodegradable nanoparticles for targeted pulmonary delivery, considering particle size, surface characteristics, tissue penetration, and regional anatomical distribution. The study is expected to establish a comprehensive morphometric database of human lungs and identify clinically relevant anatomical variations. Correlation of pulmonary dimensions and segmental anatomy with nanoparticle characteristics may provide a framework for developing anatomically informed strategies for targeted pulmonary drug delivery. Integration of pulmonary morphometry with nanotechnology may represent an emerging interdisciplinary approach in anatomical research. Understanding anatomical variations and regional pulmonary architecture could contribute to the rational design of nanoparticle-based therapies, particularly for localized pulmonary diseases, and may provide a foundation for future experimental and translational research.

Keywords: Lung morphology; Pulmonary morphometry; Nanotechnology; Nanoparticles; Drug delivery; Bronchopulmonary segments; Thoracic anatomy; Precision medicine.

Nanoparticle-Based Fluorescence Mapping of the Recurrent Laryngeal Nerve and Parathyroid Glands During Thyroid Surgery

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Abstract

Thyroid surgery is one of the most frequently performed endocrine surgical procedures. Despite advances in surgical techniques, complications such as recurrent laryngeal nerve injury, hypoparathyroidism, and incomplete identification of malignant thyroid tissue remain clinically significant. Nanotechnology offers emerging opportunities for improving intraoperative visualization, targeted diagnosis, drug delivery, and tissue preservation. To explore the potential application of nanotechnology in thyroid surgery for enhanced identification of thyroid malignancy, improved intraoperative localization of critical anatomical structures, and reduction of postoperative complications. A prospective experimental and translational study may be designed to evaluate a biocompatible nanoparticle-based imaging or contrast agent for intraoperative identification of thyroid neoplastic tissue and adjacent critical structures. Thyroid tissue specimens and, where appropriate, experimental models may be assessed using nanoparticle-mediated fluorescence or targeted molecular imaging. Histopathological findings, nanoparticle uptake, tumor-to-background contrast, and anatomical localization of the recurrent laryngeal nerve and parathyroid glands may be correlated with conventional surgical and histological findings. Nanotechnology-based targeted imaging is expected to improve differentiation between neoplastic and normal thyroid tissue and potentially enhance visualization of anatomically important structures during thyroidectomy. Improved tissue discrimination may facilitate more precise surgical resection while minimizing injury to the recurrent laryngeal nerves and parathyroid glands. Nanotechnology represents a promising frontier in precision thyroid surgery. Integration of nanomaterials with molecular targeting and intraoperative imaging could potentially transform conventional thyroidectomy into a more precise, anatomy-guided and personalized surgical procedure. Further preclinical and clinical studies are required to establish the safety, biocompatibility, diagnostic accuracy, and clinical feasibility of these approaches.

Keywords: Thyroid surgery; Nanotechnology; Thyroid carcinoma; Nanoparticles; Recurrent laryngeal nerve; Parathyroid gland; Targeted imaging; Precision surgery.

Anthropometric and Morphometric Assessment of Human Joints for Personalized Nanotechnology-Based Orthopaedic Applications

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Abstract

Accurate assessment of joint dimensions and anatomical variability is essential for understanding biomechanics, implant selection, reconstructive procedures, and development of personalized orthopaedic interventions. Nanotechnology has emerged as a promising approach in orthopaedics through the development of nanostructured implants, drug-delivery systems, and scaffolds for cartilage and bone regeneration. However, the relationship between individual joint anthropometry and the design of nanotechnology-based orthopaedic applications remains insufficiently explored. To evaluate the anthropometric and morphometric characteristics of selected human joints and explore their potential application in the development of personalized nanotechnology-based orthopaedic interventions. A cross-sectional anatomical study will be conducted to document joint-specific anthropometric and morphometric parameters. Measurements including articular surface dimensions, length, breadth, depth, curvature, and relevant anatomical indices will be obtained from selected joints using standardized osteometric techniques and/or radiological imaging. Three-dimensional reconstruction may be used to characterize joint morphology and identify anatomical variations. The morphometric data will subsequently be utilized to explore the suitability of different nanostructured biomaterials or nanoparticle-based systems for personalized implant design, cartilage regeneration, or localized therapeutic delivery. The study is expected to establish a comprehensive database of joint anthropometry and identify clinically relevant variations in articular morphology. Integration of these measurements with nanotechnology-based biomaterial design may facilitate development of anatomically compatible, patient-specific orthopaedic implants and regenerative strategies. Combining anatomical anthropometry with nanotechnology represents a promising interdisciplinary approach to precision orthopaedics. Anatomically informed nanostructured biomaterials and personalized implant designs may improve biomechanical compatibility, tissue integration, and therapeutic outcomes. Further biomechanical, experimental, and clinical studies are required to validate these applications.

Keywords: Joint anthropometry; Morphometry; Nanotechnology; Nanomaterials; Orthopaedic implants; Cartilage regeneration; 3D reconstruction; Precision orthopaedics.

IGF-1 Binding Affinity and HepG2 Cytotoxicity of *Dendrophthoe falcata* Leaf Extract: A Preliminary in Silico and *In Vitro* Evaluation of Anticancer Potential

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Abstract

Hepatocellular carcinoma (HCC) remains a leading cause of cancer mortality worldwide, and the insulin-like growth factor-1 receptor (IGF-1R) pathway is a recognized therapeutic target in liver cancer. This study presents a preliminary in silico and in vitro evaluation of the anticancer potential of a methanolic *Dendrophthoe falcata* leaf extract against HepG2 cells. Molecular docking (AutoDock Vina; PDB 1IMX, the IGF-1 crystal structure) evaluated thirteen *D. falcata* phytochemicals plus two reference compounds against IGF-1, and an MTT assay (1-1000 µg/mL) assessed HepG2 cytotoxicity. Quercetin and quercitrin engaged a hydrogen-bonded surface on IGF-1's C-domain (THR41, GLU46, ARG50/56, ASP53, ARG55) also occupied by the reference compound silibinin, silymarin's marker constituent, while the triterpenoids oleanolic acid and stigmasterol scored more negatively overall but formed almost no hydrogen bonds, instead engaging a separate, hydrophobic surface. The extract produced dose-dependent cytotoxicity ($IC_{50} = 257.4 \mu\text{g/mL}$) with a modest, plateauing effect rather than a classical sigmoidal response. These findings indicate *D. falcata* leaf extracts contain flavonoids, particularly quercetin and quercitrin, that form specific, hydrogen-bonded contacts with IGF-1 at a surface shared with a known reference compound, alongside modest HepG2 cytotoxicity, together providing preliminary support for further investigation of *D. falcata* as an anticancer agent source.

Keywords: *Dendrophthoe falcata*; IGF-1; Molecular docking; MTT assay; HepG2; Flavonoids; Quercitrin; Anticancer activity and Hepatocellular carcinoma; SDG-3

Ginger-Mediated Green Synthesis of TiO₂ Nanoparticles for Photocatalytic Removal of Pharmaceutical Pollutants

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Abstract

The increasing presence of pharmaceutical residues in water has become an important environmental concern, as conventional wastewater treatment methods may not completely eliminate many drug molecules. Nanotechnology offers promising approaches for addressing this problem, particularly through the photocatalytic properties of titanium dioxide (TiO₂) nanoparticles. The present project focuses on the green synthesis of TiO₂ nanoparticles using ginger root extract *Zingiber officinale* as a plant-based source. Ginger contains naturally occurring phytochemicals, including phenolic and antioxidant compounds, which may act as reducing, capping, and stabilizing agents during nanoparticle synthesis. A suitable titanium precursor will be combined with ginger extract under controlled experimental conditions, followed by drying and thermal treatment to obtain TiO₂ nanoparticles. The synthesized nanoparticles will be characterized using UV–Visible spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), and Scanning Electron Microscopy/Transmission Electron Microscopy (SEM/TEM) to evaluate their optical properties, functional groups, crystalline structure, morphology, and particle size. The prepared TiO₂ nanoparticles will then be investigated for their photocatalytic ability to degrade a selected pharmaceutical contaminant in water under controlled light conditions. The degradation efficiency will be evaluated by monitoring the reduction in contaminant concentration at different treatment intervals. This approach integrates green synthesis, nanotechnology, pharmaceutical science, and environmental protection. The study may provide a simple and potentially more environmentally friendly route for preparing TiO₂ nanoparticles and demonstrate their possible application in reducing pharmaceutical pollutants in wastewater. Further investigation will be required to evaluate degradation products, nanoparticle recovery, reusability, and environmental safety before practical application.

Keywords: TiO₂ nanoparticles; *Zingiber officinale*; Ginger root extract; Green synthesis; Photocatalytic degradation; Pharmaceutical wastewater.

**Bismuth oxybromide-green synthesized ZnO 3d microsphere
nanocomposite for degradation of Carbamazepine**

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Abstract

The widespread presence of ciprofloxacin (CIP) in wastewater demands sustainable remediation technologies. This study presents the facile one-pot synthesis of a novel Ag/Biochar/g-C₃N₄ ternary nanocomposite for efficient photocatalytic degradation of CIP. Agricultural waste-derived biochar and graphitic carbon nitride (g-C₃N₄) were integrated with silver (Ag) nanoparticles to construct a robust heterojunction. Comprehensive structural and optical characterization confirmed the successful synthesis of the composite. Under visible-light irradiation, the Ag/Biochar/g-C₃N₄ nanocomposite demonstrated significantly superior CIP degradation efficiency compared to pristine g-C₃N₄ and binary counterparts. This enhanced activity is attributed to a powerful synergistic effect: Ag nanoparticles broaden visible-light absorption via surface plasmon resonance, while highly conductive biochar facilitates rapid electron transfer, minimizing the recombination of photo-generated electron-hole pairs. The highly stable and reusable ternary composite offers an eco-friendly, high-performance solution for the sustainable treatment of antibiotic-contaminated wastewater.

Keywords: g-C₃N₄, Biochar, Silver nanoparticles, Ciprofloxacin.

Phytogetic Gold Nanoparticles Using *Clitoria Ternatea*: A Green Nanomedicine Approach for Breast Cancer Research

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Abstract

Breast cancer is one of the major global health challenges, creating a continuous need for safer, effective, and sustainable therapeutic approaches. Green nanotechnology provides an eco-friendly alternative to conventional nanoparticle synthesis by utilizing biological resources as reducing and stabilizing agents. *Clitoria ternatea* (Butterfly pea) is a phytochemically rich medicinal plant containing flavonoids, anthocyanins, and other bioactive constituents that may facilitate nanoparticle synthesis and contribute to biological activity. The present study aims to develop gold nanoparticles (AuNPs) using *Clitoria ternatea* flower extract through a green synthesis approach and to investigate their preliminary in vitro anticancer potential against breast cancer cells. Authenticated butterfly pea flowers will be processed to prepare a standardized aqueous extract, which will be reacted with a suitable gold precursor under optimized conditions for nanoparticle formation. The synthesized AuNPs will be characterized using UV–Visible spectroscopy, Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), electron microscopy, dynamic light scattering (DLS), and zeta-potential analysis to determine their optical, structural, morphological, and colloidal properties. The biological activity will be evaluated using a concentration-dependent cell viability assay against an appropriate breast cancer cell model, along with suitable controls. Where feasible, oxidative stress and apoptosis-related parameters will be assessed to provide preliminary insights into the possible mechanism of action. The study is expected to establish a sustainable plant-mediated route for AuNP synthesis and generate preliminary evidence regarding their potential anticancer activity. Further studies on selectivity, toxicity, mechanistic pathways, and in vivo efficacy will be required to establish their future therapeutic potential.

Keywords: *Clitoria ternatea*; Butterfly pea; Gold nanoparticles; Green synthesis; Breast cancer; Nanomedicine; Phytochemicals; Cytotoxicity; Apoptosis

Isolation, Characterization, and *In Vitro* Evaluation of Epiphyllum oxypetalum Against Human Breast Cancer Cells

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Abstract

This study evaluated the in vitro anticancer efficacy of bioactive constituents isolated from Epiphyllum oxypetalum against MDA-MB-231 human breast adenocarcinoma cells. Ethanolic crude extracts were fractionated chromatographically and characterized via GC-MS and HPLC, confirming the presence of flavonoids, phenolic, steroids, and terpenoids. Cytotoxicity and selectivity were assessed using the MTT assay on MDA-MB-231 and normal control cells. The isolated fractions demonstrated significant, concentration-dependent ant proliferative activity with low IC₅₀ values and hallmark apoptotic features (cell shrinkage, membrane blebbing, and nuclear fragmentation) while exhibiting minimal toxicity to normal cells. These findings highlight E. oxypetalum as a promising source of selective antineoplastic agents against breast cancer.

Antioxidant And Antibacterial Activity of *Apium Graveolens* Leaves (*Celery Leaves*) In Hexane Extract

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Abstract

The Present study investigates the Antioxidant and Antibacterial activity of the hexane extract of *Apium graveolens* (celery) leaves. Celery (*Apium graveolens* L.) is a highly nutritious plant and part of a healthy diet, as it is considered a good source of biologically-active compounds, such as carotenes, tocopherols, flavonoids, alkaloids, terpenoids, and phenolic acids. Due to its broad biological activity, celery prevents and heals numerous ailments, including asthma, cardiovascular, liver, and spleen diseases, gastrointestinal disorders, increases male fertility, and different types of cancer. The extract showed higher phenolic content and stronger antioxidant activity in the Ferric reducing antioxidant power test, and also exhibited antimicrobial activity against *Staphylococcus aureus*, *Salmonella typhi* and *Aspergillus flavus*. The antioxidant activity was evaluated using the DPPH assay, showing a concentration-dependent increase in free radical scavenging activity. The antibacterial activity tested against *Escherichia coli* demonstrated a zone of inhibition at higher concentrations, indicating its antimicrobial potential. Overall, the study suggests that *Apium graveolens* leaves possess significant bioactive properties and can serve as a potential natural source of antioxidant and antibacterial agents.

Key words: *Apium graveolens*, *Staphylococcus aureus*, *Salmonella typhi* and *Aspergillus flavus*, *Escherichia coli*.

Hydrothermal Synthesis and Characterization of Ni-AgO Core-Shell Nanoparticles: A Potent Application Towards Against Hepg2 Human Hepatocellular Carcinoma Cells

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Abstract

Nickel-doped silver oxide (Ni-AgO) core-shell nanoparticles were successfully synthesized by hydrothermal method using AgNO₃ and NiCl₂ at Ni:Ag = 55:45 molar ratio with NaOH at 120–150°C for 12–18 hours. XRD confirmed the FCC crystalline phase (JCPDS: 87-0719) with planes at (111), (200), (220), and (311). FE-SEM revealed spherical core-shell morphology, TEM gave an average particle size of 60.25 ± 7.6 nm, HRTEM showed resolved lattice fringes, and SAED confirmed polycrystalline FCC phase. UV-Vis showed absorption at 317 nm and 358 nm; FTIR confirmed Ag–O (579 cm⁻¹) and Ni–O (480 cm⁻¹) stretching vibrations. MTT cytotoxicity against HepG2 cells gave IC₅₀ = 315.19 µg/mL (24 h). DAPI staining, AO/EtBr dual staining, and H₂DCFDA ROS assay collectively confirmed ROS-mediated intrinsic apoptosis as the primary cytotoxic mechanism. Antibacterial evaluation by agar well diffusion showed selective activity against Staphylococcus aureus (ZOI: 10–13 mm at 25–100 µg/mL) with Levofloxacin as standard (25 mm), while Pseudomonas aeruginosa was inhibited only at 100 µg/mL (ZOI: 11 mm; Ciprofloxacin standard: 33 mm). These results establish Ni-AgO core-shell nanoparticles as promising multifunctional nanomaterials with anticancer, apoptotic, pro-oxidant, and antibacterial activities.

Keywords: Ni-AgO, HepG2, DAPI, AO/EtBr, antibacterial

One-Pot Construction of a Novel Morpholine–Furfuraldehyde Functionalized Maleimide: Spectral Characterization

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Abstract

Mannich bases constitute an important class of bioactive organic compounds with diverse pharmaceutical and coordination chemistry applications. In the present study, a novel Mannich base, N-(morpholinomethyl) maleimide (MOMM), was synthesized by a one-pot Mannich condensation of maleimide, morpholine, and formaldehyde in a 1:1:1 molar ratio under mild reaction conditions. The synthesized compound was obtained as a white crystalline solid with a 62% yield and a melting point of 77 °C after recrystallization from ethanol. The structure of MOMM was comprehensively characterized using elemental (CHN) analysis, UV-Visible spectroscopy, FT-IR, ¹H NMR, ¹³C NMR, and mass spectrometry. Elemental analysis was consistent with the proposed molecular formula C₁₃H₁₄N₂O₃. The UV–Visible spectrum exhibited characteristic $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions of the maleimide chromophore. FT-IR spectral studies confirmed the disappearance of N–H stretching vibrations of the starting materials and the appearance of characteristic imide carbonyl and C–N–C stretching bands, indicating successful Mannich condensation. The ¹H NMR spectrum displayed a distinct N–CH₂–N methylene signal along with characteristic morpholine and olefinic proton resonances, while the ¹³C NMR spectrum further established the presence of carbonyl, olefinic, morpholine, and methylene carbons. The molecular ion peak observed at m/z 196 in the mass spectrum agreed well with the calculated molecular weight, confirming the formation of the desired product. The combined spectral and analytical data conclusively establish the successful synthesis and structural elucidation of MOMM. The synthesized ligand serves as a promising precursor for the preparation of transition metal complexes and warrants further investigation for its biological and coordination properties.

Keywords: Mannich base; Maleimide; Morpholine; N-(morpholinomethyl)maleimide; Spectral characterization; FT-IR; NMR; Mass spectrometry.

Targeting Sickle Haemoglobin through the Rapid Green Synthesis of Coumarin–Pyrazole Hybrids Using a Synergistic Ultrasonic–Micellar–Nanoparticle Nanoreactor

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Abstract

Sickle cell disease (SCD) stands as one of the most widespread inherited haematological disorders globally, driven by the polymerization of deoxygenated sickle haemoglobin (HbS). Developing novel anti-sickling therapeutics with high efficacy and minimized adverse side effects remains an essential objective. Herein, we report the first green, highly efficient, and synergistic micellar nano-catalytic strategy for the synthesis of a structurally diverse library of novel 4-(5-hydroxy-3-methyl-1H-pyrazol-4-yl) chroman-2-one derivatives (3 series) by hybridizing coumarin and pyrazole pharmacophores. To overcome the long reaction times (1080–2880 min.) and ring-opening limitations associated with conventional organic solvent methods, the Michael cyclization sequence was optimized using gemini-based aqueous micellar medium combining semiconductor nanoparticles (CdS-g4 or PbS-g5) under ultrasound irradiation (100 W). The optimized integrated protocol utilizing 0.020 wt% PbS-g5 NPs in g5 micellar solution accelerated the reaction rate, dropping the time down to just 20 min. at room temperature, while, delivering good yields (77–92%). Both nanocatalysts demonstrated high operational stability and were efficiently recycled over three consecutive runs with minimal loss of activity. Evaluated, *in vitro*, against sodium metabisulfite-induced erythrocyte sickling and HbS polymerization assays, the target hybrids displayed prominent, concentration-dependent anti-sickling activity. Notably, compounds 3 and 3a emerged as the most potent candidates, demonstrating better morphological restoration of red blood cells and robust suppression of HbS fiber formation, closely mirroring the clinical reference drug hydroxyurea. Furthermore, molecular docking simulations against deoxyhaemoglobin S (PDB ID: 5E83) corroborated the, *in vitro*, results, revealing better binding complementarities (docking scores up to -8.4 kcal·mol⁻¹) stabilized by a dense network of hydrogen bonding, electrostatic, and hydrophobic interactions (e.g., Lys99, Ser133, and Asp126). Overall, the present study combines green nanotechnology with medicinal chemistry to generate coumarin–pyrazole hybrids that permit further investigation as potential antisickling agents.

Keywords: Coumarin–pyrazole hybrids; Gemini surfactant as micellar medium; Semiconductor nanoparticles; Ultrasound-assisted synthesis; Anti-sickling activity; Deoxyhaemoglobin S.

Analysis of PLA-Based 3D-Printed Hybrid Functional Polymer Composite for Structural Applications

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Abstract

The 3D printing process is one of the finest manufacturing techniques in the development of complex shapes with decent quality. Currently, this technique is widely applied for biomedical, automobile and aerospace applications. Though the fused deposition modelling (FDM) is accepted, the material selection is a crucial challenge, which depends on the material flow index (MFI) of the developed filament. Since industries are developing new kinds of composite material that must fit for the 3D printing process, it is necessary to do research in developing advanced functional polymer composites to replace the conventional polymer materials. In this work, a novel hybrid polymer filament was developed with PLA matrix and nano-sized reinforcements like barium titanate (BTO) and cobalt ferrite (CoFe_2O_4) by means of a pelletization process and extruded through the twin extruder machine. To identify the suitability of this filament for structural applications, it was further printed with Ender 3 Max m/c following FDM method and tested as per the ASTM standards. The tensile results showed that the printed sample (ASTM D638) of the hybrid functional composite showed a maximum of 40 MPa ultimate tensile strength (UTS) with decent ductility when compared with PLA sample without the reinforcements. The SEM and EDS results of the filament showed the good bonding between matrix and reinforcement with the elements of 'Ti', 'Ba', 'Co' and 'Fe'. The addition of reinforcement is limited to 5% to avoid the maximum agglomeration and to reduce the breaking of filament during the extrusion.

Keywords: 3D printing, hybrid filament, BTO, CoFe_2O_4

Impact Of Pharmaceutical Care on Medication Adherence and Quality of Life Among Breast Cancer Patients Undergoing Chemotherapy

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Abstract

Background: Breast cancer patients undergoing chemotherapy frequently experience impaired quality of life (QoL) and difficulties with medication adherence due to complex treatment regimens, treatment-related adverse effects, and inadequate understanding of medication use. Pharmaceutical care provided by clinical pharmacists, including patient education and medication counseling, may help patients better understand and manage their therapy, thereby improving treatment outcomes. The present study was undertaken to evaluate the impact of clinical pharmacist-mediated pharmaceutical care on quality of life and medication adherence among breast cancer patients receiving chemotherapy. **Methodology:** A prospective interventional study was conducted in the Department of Radiotherapy and Oncology at Salem Zone, Tamil Nadu, among 172 breast cancer patients undergoing chemotherapy. Participants were randomly allocated into a control group (n=130) and an intervention group (n=130). Patients in the intervention group received pharmaceutical care comprising medication counseling and patient education using validated Patient Information Leaflets (PILs). Two PILs were developed, validated, translated, and evaluated for user acceptability. Quality of life was assessed at baseline, mid-treatment, and end-treatment using the European Organisation for Research and Treatment of Cancer Quality of Life Questionnaire-C30 (EORTC QLQ-C30) and the breast cancer-specific QLQ-BR23 questionnaire. Medication adherence was assessed using the Morisky, Green, and Levine (MGL) adherence scale. **Results:** At baseline, no statistically significant differences were observed between the intervention and control groups in the functional and symptom domains of the EORTC QLQ-C30. Following the pharmaceutical care intervention, significant improvements were observed in the intervention group in role functioning (p<0.001), emotional functioning (p<0.001), cognitive functioning (p<0.001), and social functioning (p=0.027) at the first follow-up. By the second follow-up, a significant improvement was also observed in global health status/QoL (p<0.001). Among the symptom domains, significant reductions in fatigue (p=0.001) and insomnia (p=0.003) were observed in the intervention group at the first follow-up and were maintained at the subsequent assessment. Assessment using the EORTC QLQ-BR23 demonstrated significant improvements in body image and future perspective at both follow-ups (p<0.001). At the second follow-up, significant reductions were also observed in arm symptoms (p=0.004) and distress related to hair loss (p<0.001) among patients receiving pharmaceutical care. Medication adherence scores were comparable between the groups at baseline; however, adherence improved progressively during follow-up, with a greater improvement observed in the intervention group. **Conclusion:** Clinical pharmacist-mediated pharmaceutical care, incorporating structured patient education, medication counseling, and validated Patient Information Leaflets, significantly improved quality of life and medication adherence among breast cancer patients undergoing chemotherapy. The intervention enhanced patients' understanding of their treatment and supported better management of treatment-related symptoms. These findings highlight the important role of clinical pharmacists as integral members of the oncology care team and support the incorporation of pharmaceutical care services into routine cancer care to improve patient-centered outcomes.

Keywords: Breast cancer; Chemotherapy; Clinical pharmacist; Medication adherence; Pharmaceutical care; Patient education; Quality of life.

Synergistic Co-Delivery of Anthocyanins and Indole-3-Propanoic Acid via a Biogenic Cellulose Matrix for Anti-inflammation, Anti-oxidant therapy

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Abstract

Colorectal Cancer (CRC) is a leading cause of mortality worldwide, with its pathogenesis heavily driven by chronic inflammation and oxidative stress. While natural phytochemicals such as Anthocyanins (ACN) and microbial metabolites like Indole-3-propanoic acid (IPA) offer significant therapeutic potential, their clinical efficacy is often restricted by poor stability and low bioavailability. To address this challenge, the present study developed a novel bioactive composite, MC-BO-IPA, by encapsulating these agents within a porous Microcrystalline Cellulose (MCC) carrier sustainably synthesized from *Luffa cylindrica*. Physicochemical characterization via X-ray Diffraction (XRD) revealed that the encapsulation process successfully induced a phase transition of the bioactive payload from a crystalline to an amorphous state, thereby enhancing solubility. Scanning Electron Microscopy (SEM) confirmed a heterogeneous, "craggy" surface morphology favorable for drug release, while Fourier-Transform Infrared Spectroscopy (FTIR) and Energy Dispersive X-ray (EDX) validated the chemical integrity and successful loading of the indole and phenolic functional groups. In vitro assays demonstrated that MC-BO-IPA exhibits potent, dose-dependent antioxidant activity (up to 75% DPPH scavenging) and significant anti-inflammatory potential (60% membrane stabilization). Furthermore, antiproliferative studies on the HT-29 colorectal cancer cell line revealed that the composite exerts selective cytotoxicity through ROS-mediated apoptosis, evidenced by mitochondrial membrane potential loss and nuclear fragmentation. These findings establish MC-BO-IPA as a promising, "green" therapeutic candidate that leverages the synergistic properties of plant-derived polymers and bioactive metabolites for the targeted management of colorectal cancer.

Keywords: Microcrystalline cellulose, *Luffa cylindrica*, Antioxidant activity, Anticancer activity, Ros generation.

Formulation and Optimization of Probiotic Jelly from Royal Jelly, Estimation and Evaluation of Its Viability, Nutrients and Sensory Properties

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Abstract

In the jelly, the royal jelly was formulated and optimized at different concentrations such as royal jelly in 10, 20, 30, 40, and 50%, and in each sample, citric acid was added 2 drops and gelatin 0.6 gm for production. Jellies were analysed qualitatively and quantitatively and sensory attributes were to find the most suitable composition for commercialization. On the basis of the conclusion sample 3 with 0.6 gm of gelatin, 2 drops of citric acid and 30 ml of royal jelly was chosen as best and in the sample, the *Lactobacillus acidophilus* was added and the viability was evaluated every 4 days after inoculation of a probiotic organism to the developed jelly. The number of colonies were increased every 4 days. At the end of 20th day 160 colonies were formed.

Keywords: Royal jelly, gelatin, *Lactobacillus acidophilus*, viability, colonies, probiotic jelly, colony-forming units

Biosynthesis and Characterization of Solenopsis Invicta Protein Rich Extract Coated Selenium Nanoparticles and Evaluation of Their Antioxidant Activity

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Abstract

Prostate cancer is one of the most prevalent malignancies among men worldwide and is closely associated with oxidative stress, redox imbalance, and resistance to apoptosis. In recent years, green nanotechnology has gained attention as a strategy to develop biocompatible and eco-friendly therapeutic materials. The present study aimed to synthesize selenium nanoparticles (SeNPs) using a protein-rich homogenate of *Solenopsis invicta* (fire ant) as a natural reducing and stabilizing agent, and to evaluate their physicochemical characteristics, antioxidant potential, and anticancer efficacy against PC3 human prostate cancer cells. Ant protein-rich extract-derived SeNPs (AE-SeNPs) were synthesized via a protein-mediated green route, confirmed by a visible color change from pale yellow to deep orange-red. UV–Visible spectroscopy showed a characteristic absorption peak at 265 nm. X-ray diffraction analysis confirmed the crystalline trigonal structure of elemental selenium, while FTIR spectroscopy revealed the involvement of protein and chitin-associated functional groups in nanoparticles (NPs) capping and stabilization. SEM analysis demonstrated predominantly spherical NPs in the nanoscale range, and EDX confirmed selenium as the major elemental component with organic capping. The SeNPs showed a near-neutral zeta potential (–0.1 mV) and negligible electrophoretic mobility, suggesting limited electrostatic stabilization and a tendency toward NPs aggregation in suspension. In antioxidant assays, the crude ant extract exhibited stronger radical scavenging activity than AE-SeNPs, with IC₅₀ values of 60.57 µg/mL (DPPH) and 28.21 µg/mL (ABTS), whereas AE-SeNPs showed IC₅₀ values of 368.80 µg/mL and 378.13 µg/mL, respectively. Overall, this study demonstrates that ant-derived protein-coated SeNPs can be synthesized through a sustainable green approach and exhibit promising physicochemical stability and selective anticancer potential, highlighting their relevance as eco-friendly nanotherapeutic candidates for prostate cancer management.

Keywords: Fire ant extract, SeNPs, Prostate cancer, green synthesis, Antioxidant activity, spectroscopy

Synergistic Co-Delivery of Anthocyanins and Indole-3 Propanoic Acid via a Biogenic Cellulose Matrix for Colorectal Cancer Therapy

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Abstract

Colorectal Cancer (CRC) is a leading cause of mortality worldwide, with its pathogenesis heavily driven by chronic inflammation and oxidative stress. While natural phytochemicals such as Anthocyanins (ACN) and microbial metabolites like Indole-3- propanoic acid (IPA) offer significant therapeutic potential, their clinical efficacy is often restricted by poor stability and low bioavailability. To address this challenge, the present study developed a novel bioactive composite, MC-BO-IPA, by encapsulating these agents within a porous Microcrystalline Cellulose (MCC) carrier sustainably synthesized from *Luffa cylindrica*. Physicochemical characterization via X-ray Diffraction (XRD) revealed that the encapsulation process successfully induced a phase transition of the bioactive payload from a crystalline to an amorphous state, thereby enhancing solubility. Scanning Electron Microscopy (SEM) confirmed a heterogeneous, "craggy" surface morphology favorable for drug release, while Fourier-Transform Infrared Spectroscopy (FTIR) and Energy Dispersive X-ray (EDX) validated the chemical integrity and successful loading of the indole and phenolic functional groups. In vitro assays demonstrated that MC-BO-IPA exhibits potent, dose-dependent antioxidant activity (up to 75% DPPH scavenging) and significant anti-inflammatory potential (60% membrane stabilization). Furthermore, antiproliferative studies on the HT-29 colorectal cancer cell line revealed that the composite exerts selective cytotoxicity through ROS-mediated apoptosis, evidenced by mitochondrial membrane potential loss and nuclear fragmentation. These findings establish MC-BO-IPA as a promising, "green" therapeutic candidate that leverages the synergistic properties of plant-derived polymers and bioactive metabolites for the targeted management of colorectal cancer.

Keywords: Microcrystalline cellulose, *Luffa cylindrica*, Anticancer activity, Ros generation.

Yttrium-substituted Ni-Zn spinel ferrites: Structural evolution and enhanced visible light photocatalytic and antimicrobial activity

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Abstract

Yttrium (Y³⁺) substituted nickel-zinc spinel ferrites, $\text{Ni}_{0.9}\text{Zn}_{0.1}\text{Y}_x\text{Fe}_2\text{O}_4$ ($x = 0.00-0.10$), were synthesized using the citrate sol-gel auto-combustion technique and their structural, surface-chemical, optical, magnetic, photo-catalytic, antibacterial and antifungal properties were extensively examined. X-ray diffraction confirmed the predominance of the cubic spinel $\text{Fd}\bar{3}\text{m}$ phase, while Rietveld refinement revealed minor orthorhombic yttrium orthoferrite at $x \geq 0.06$, reaching 4.58 wt% in NZYF10. FESEM and HRTEM analyses revealed aggregated, near-spherical nanocrystals, and EDX confirmed the expected stoichiometric composition. XPS analysis confirmed the surface elemental composition and composition-dependent chemical-state environments. UV-Vis diffuse-reflectance analysis revealed a monotonic decrease in the optical band-gap energy from 1.98 eV for NZF to 1.55 eV for NZYF10, indicating enhanced visible-light absorption. Photoluminescence revealed composition-dependent emissive relaxation, while EIS showed a smaller interfacial impedance response for NZYF10 than for NZYF8, supporting more favourable interfacial charge transfer in NZYF10. Magnetic experiments (VSM) revealed composition-dependent fluctuations in saturation magnetization and coercivity, attributable to cation redistribution and modification of magnetocrystalline anisotropy. NZYF10 exhibited the highest methyl-orange degradation efficiency of 68.53% under visible-light irradiation, following pseudo-first-order kinetics. The enhanced activity was associated with improved visible-light absorption, favourable interfacial charge transfer, and accessible surface reaction sites. Antimicrobial and antifungal tests showed a composition-dependent inhibitory behaviour. Bacterial strains were shown to be more susceptible than fungal strains. The results demonstrate that nominal Y substitution effectively tailors the structure, defect chemistry, and functional properties of Ni-Zn ferrites, establishing meaningful structure-defect-property relationships. NZYF10 shows promising potential as a multifunctional material for visible-light-driven environmental remediation and antibacterial applications.

An Explainable, Threshold-Optimized XGBoost Framework for Parkinson's Disease Detection from Sustained-Vowel Vocal Biomarkers

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Abstract

Parkinson's disease (PD) is a progressive neurodegenerative disease which continues to have an unmet clinical need for early, low cost, non-invasive screening. In this paper, an end-to-end explainable machine learning (XAIME) pipeline for detecting PD from sustained-vowel acoustics recordings is presented. The pipeline consists of correlation-based filtering, L1 regularization and Recursive Feature Elimination (RFE), feature selection using SHapley Additive exPlanations (SHAP), class balancing using Synthetic Minority Oversampling Technique (SMOTE) and Standard Scaler normalization. An XGBoost classifier with eight SHAP-selected biomarkers correctly identified 28 of 29 PD cases with a 92.31% accuracy, 93.33% precision, 96.55% recall, a 94.92% F1-score and a 97.24% ROC-AUC on held-out test data. Decision-threshold optimization (0.50 $\rightarrow$ 0.10) further brought accuracy up to 97.24%. Training-convergence and ROC-curve analysis shows stable learning and consistent discrimination improvement over the untuned XGBoost baseline (82.05% accuracy, 88.62% ROC-AUC) and a hyperparameter-tuned variant which showed mild overfitting. In addition, the proposed static screening model is compared to upcoming digital-twin (DT) concepts for PD monitoring, demonstrating their complementary nature: the proposed model provides immediate deployable, interpretable screening from a single recording while DT models are geared towards longitudinal personalized monitoring but have not yet been validated for PD. The results indicate that the proposed multi-stage feature selection approach, combined with SHAP interpretability and clinically motivated threshold calibration, results in a high-sensitivity screening tool that is easy to interpret and can support clinical decision-making.

Keywords: Parkinson's disease, vocal biomarkers, XGBoost, SHAP, explainable AI, feature selection, SMOTE, class imbalance, threshold optimization, ROC curve, digital twin

Optimisation and Characterization of Neem Gum- Carboxymethyl Cellulose Composite Biodegradable Films Using Box-Behnken Response Surface Methodology

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Abstract

The widespread use of petroleum-based plastics in food packaging has contributed significantly to environmental pollution, creating an urgent need for sustainable biodegradable materials derived from renewable natural resources. Among them, neem gum (*Azadirachta indica*) a natural polysaccharide possesses excellent film-forming potential and its application in biodegradable food packaging has received limited scientific attention. Therefore, the present study aimed to develop and optimize neem gum-carboxymethyl cellulose (CMC) composite biodegradable films plasticized with glycerol using Response Surface Methodology (RSM) based on a three-factor, three-level Box-Behnken experimental design. The effects of neem gum, CMC, and glycerol concentrations on film thickness, moisture content, and elongation at break were optimized, and the developed models were validated experimentally. The optimized formulation produced a biodegradable film with a thickness of 0.700 ± 0.04 mm, tensile strength of 0.238 MPa, elongation at break of 84.90%, and water solubility of 32.15%. Characterization of the optimized film revealed a stable polymer network with strong intermolecular interactions, a predominantly amorphous structure, and a compact, homogeneous surface morphology. The film also exhibited desirable thermal stability and barrier properties, supporting its suitability for biodegradable food packaging applications. These findings demonstrate that neem gum is a promising renewable biopolymer for sustainable packaging materials and provide a strong foundation for future research on functional biodegradable films.

Keywords: Neem gum, Carboxymethyl cellulose, Biodegradable film, Response Surface methodology, Natural Polysaccharide, Sustainable food packaging.

Corrosion Study of Aluminium Steel is in Contact with Acid Medium using Expired Labetalol Drug (ELT) as Inhibitor

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Abstract

The corrosion inhibitive action of expired Labetalol drug (ELT) on the corrosion of aluminium steel in 1N HCl medium has been evaluated at room temperature by weight loss method. The weight loss measurements showed that corrosion inhibition efficiency increased on increasing the concentration of the inhibitor and maximum protection efficiency at 250 ppm. The mechanistic aspects of corrosion resistance have been studied by potentiodynamic polarization technique and electrochemical impedance spectroscopy (EIS). Potentiodynamic polarization technique reveals that the inhibitor system functions as mixed type of inhibitor, controlling anodic and cathodic reactions preferably. It is noted that in presence of inhibitor, linear polarization resistance value increases, and corrosion current decreases. Electrochemical impedance studies reveal that a protective film (blanket effect) is formed on the aluminium steel surface, since in the presence of inhibitor system the charge transfer resistance value increases and double layer capacitance value decreases. FTIR spectra were utilized to identify bonds of ELT on aluminium steel surface and pure expired drug. The surface morphology of inhibited aluminium steel was analyzed by scanning electron microscope (SEM) and atomic force microscopy (AFM). The results have clearly shown that ELT has the inhibiting capacity for reducing the corrosion of aluminium steel immersed in acid medium.

Keywords: Acidic solutions, Aluminium steel, AFM, Labetalol, Corrosion inhibitor and SEM.

Bioactivity Assessment of Zinc Oxide Nanoparticles with Enhanced Antibacterial and Antioxidant Potential

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Abstract

Nanotechnology enables the design, development, and engineering of materials at the nanoscale level enabling the generation of unique physicochemical properties and functionalities. Research has demonstrated that nanotechnology offers significant potential for the development of advanced antimicrobial materials by minimizing antimicrobial consumption, enhancing antimicrobial effectiveness, improving environmental sustainability, and contributing to better material quality and performance. Zinc Oxide nanoparticles (ZnO-NPs) are recognized for their antibacterial and antifungal properties. Here ZnO-NPs were synthesized by sol-gel method for assessment of antibacterial and antioxidant potential. The nanoparticles were characterized by SEM, FTIR and PXRD. Scanning Electron Microscopy images show the synthesized ZnO-NPs are spherical though some agglomerated into undefined shapes. FTIR analysis showed peaks at 430 cm^{-1} , 1380 cm^{-1} , and 3440 cm^{-1} . The ZnO-NPs showed an optical band gap of 3.395 eV and a zeta potential of $-17.1 \pm 0.95\text{ mV}$. The antioxidant activity was 94.01% (DPPH test), and antibacterial testing revealed strong inhibition against *Staphylococcus aureus* ($14.0 \pm 0.33\text{ mm}$), outperforming *E. coli* and *Streptococcus sp.* The study demonstrates the enhanced antibacterial and antioxidant potential of ZnO nanoparticles which may facilitate their potential in medicine, tissue regeneration, food, and agriculture industries.

Keywords: nanoparticles, zinc oxide, antibacterial, antioxidant, zeta-potential

Preparation and Characterization of Astaxanthin-Loaded *Moringa oleifera*-Mediated Zinc Oxide Nanoparticles

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Abstract

Zinc oxide nanoparticles (ZnO NPs) synthesized via green routes offer a sustainable, low-toxicity alternative to conventional chemical methods for biomedical and nutraceutical applications. In this study, ZnO NPs were synthesized using *Moringa oleifera* leaf extract as a natural reducing and capping agent, followed by loading with astaxanthin, a potent carotenoid antioxidant, to enhance its stability and bioavailability. *Moringa oleifera* leaves were collected, processed, and used to prepare aqueous extract, which facilitated the green synthesis of ZnO NPs. Astaxanthin was subsequently incorporated onto the nanoparticle surface. The synthesized nanoparticles were characterized using UV-Visible spectroscopy, FTIR, XRD, SEM/TEM, and zeta potential analysis to confirm formation, functional groups, crystallinity, morphology, and stability. Astaxanthin loading efficiency and release behavior were evaluated using UV-Vis/HPLC-based quantification. Results confirmed successful green synthesis of well-dispersed ZnO NPs with characteristic optical and structural properties, and effective astaxanthin loading with improved stability compared to free astaxanthin. These findings suggest that *Moringa oleifera*-mediated astaxanthin-loaded ZnO nanoparticles hold promise as a stable, eco-friendly nanocarrier system for antioxidant delivery in biomedical applications.

Keywords: Zinc oxide nanoparticles, *Moringa oleifera*, Astaxanthin, Green synthesis

Auto Combustion Mediated Cobalt Ferrite Nanoparticles for Biomedical Applications

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Abstract

Magnetic ferrite nanoparticles present their unique properties which make them suitable for several applications in biomedical field such as magnetic resonance imaging (MRI), hyperthermia and drug delivery systems. The magnetic hyperthermia treatment involves heating the cancer cells by using magnetic ferrite particles exposed to an alternating magnetic field. The cancer cell temperature increases because of the thermal propagation of the heat induced by the ferrite nanoparticles into the affected region. In order to increase the effectiveness of the treatment, hyperthermia can be combined with drug delivery techniques. As a spectroscopic technique MRI is used in medicine for the imaging of tissues especially the soft tissues and diagnosing malignant tumors. For this purpose $\text{Ni}_x\text{Co}_{1-x}\text{Fe}_2\text{O}_4$ (where $x = 0.0, 0.1, 0.2, 0.3, 0.4$) ferrite nanoparticles synthesized via solution combustion technique. The cubic spinel structure formation of ferrite phase was confirmed by X-ray diffraction analysis using synchrotron radiation. The nanocrystalline ferrite exhibits a very limited structural coherence length and a high degree of structural disorder. The ferrite nanoparticles possess a very well defined local atomic ordering that may be described in terms of a spinel-type structure with Co^{2+} and Fe^{3+} ions almost randomly distributed over its tetrahedral and octahedral sites. The new structural information helps to explain the material's unusual magnetic properties. The average grain diameter, surface morphology and microstructure of ferrite nanoparticles were studied by using SEM. The average grain diameter was found to decrease with increasing Ni content up to $x = 0.3$ and then slightly increases for $x = 0.4$. The variation of DC resistivity with temperature shows the break at Curie temperature, indicating the transition from ferromagnetism to paramagnetism. The magnetic properties of ferrites were studied by using M-H Hysteresis loop and is found to increase with increasing Ni concentration in copper ferrites.

Keywords: Solution combustion technique, magnetic resonance imaging (MRI), hyperthermia, drug delivery systems and Saturation magnetization.

Characterization and Antibacterial Activity of Bacteriocin Producing *Lactobacillus* Isolated from Bovine Colostrum Milk

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Abstract

Lactic acid bacteria LAB are a phylogenetically and functionally diverse family of gram-positive micro-organisms, known to possess beneficial probiotic-like properties. Bacteriocin-producing lactic acid bacteria are promising natural antimicrobial agents with potential applications in food preservation and safety. The present study aims to isolate and characterize *Lactobacillus* spp. from bovine colostrum milk and evaluate their bacteriocin-producing ability. The isolates will be identified based on morphological, biochemical, and microbiological characteristics, followed by screening for bacteriocin production. The antibacterial activity of the extracted bacteriocin will be assessed against selected foodborne and pathogenic bacteria using suitable antimicrobial assays. The study is expected to identify potent bacteriocin-producing *Lactobacillus* strains that may serve as natural biopreservatives and contribute to the development of safer and extended-shelf-life food products.

Key words: Antimicrobial activity, Lactic acid bacteria, Bacteriocin, Bovine Colostrum milk, Biopreservatives.

Green Nanotechnology in Oral Cancer: *Calotropis procera*-Mediated ZnO Nanoparticles and VEGFR2 Modulation

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Abstract

Oral squamous cell carcinoma remains a major health challenge, necessitating the development of innovative and biologically relevant therapeutic strategies. Green synthesis of zinc oxide nanoparticles (ZnO-NPs) using medicinal plants provides an environmentally sustainable approach that may enhance the biological activity of plant-derived compounds. This study aimed to synthesize ZnO nanoparticles using *Calotropis procera* leaf extract and evaluate their physicochemical characteristics, anticancer activity, reactive oxygen species (ROS) generation, apoptosis and VEGFR2-associated molecular response in KB oral carcinoma cells. Aqueous *C. procera* leaf extract was used as a reducing and stabilizing agent for ZnO nanoparticle synthesis. The synthesized nanoparticles were characterized using UV–visible spectroscopy, X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), field-emission scanning electron microscopy (FE-SEM), energy-dispersive X-ray spectroscopy (EDX) and zeta-potential analysis. Cytotoxicity was evaluated by MTT assay after 24 h exposure, with 5-fluorouracil (5-FU) as the reference drug. Intracellular ROS was assessed using DCFH-DA, apoptosis-associated morphological changes by acridine orange/ethidium bromide staining, and VEGFR1, VEGFR2, EGFR and NTRK expression by RT-qPCR. XRD confirmed crystalline hexagonal wurtzite ZnO with an estimated crystallite size of approximately 36 nm. FTIR indicated phytochemical capping, while EDX confirmed Zn/O composition with residual carbon. The zeta potential was –39.9 mV. CP-Zn-NP demonstrated concentration-dependent cytotoxicity with an IC₅₀ of approximately 172.6 µg/mL compared with 133.8 µg/mL for 5-FU. ROS increased approximately 3.97-fold, accompanied by apoptotic morphological changes. VEGFR2 expression decreased to approximately 0.56-fold, whereas VEGFR1, EGFR and NTRK were upregulated. *C. procera*-mediated ZnO nanoparticles demonstrated promising ROS-associated cytotoxicity, apoptotic changes and VEGFR2-modulatory effects in KB oral carcinoma cells, supporting further mechanistic and in-vivo investigation.

Keywords: *Calotropis procera*; zinc oxide nanoparticles; green synthesis; oral squamous cell carcinoma; KB cells; reactive oxygen species; apoptosis; VEGFR2; nanotechnology.

Green Synthesis of ZnO Nanoparticles Using Fish Scale Hydrolysate for Biomedical Applications

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Abstract

Zinc oxide nanoparticles (ZnO NPs) are highly versatile nanoplatforms and widely used in biomedical and cosmetic products as they have antimicrobial and antioxidant properties. Green synthesis of ZnO NPs provides an eco-friendly and sustainable substitute to conventional chemical synthesis. In the current study, Rohu (*Labeo rohita*) fish scale hydrolysate (FSH) prepared through biological hydrolysis using *Stenotrophomonas koreensis* was utilized as a stabilizing and reducing agent for the synthesis of ZnO NPs. Characterization of ZnO NPs was performed using UV–visible spectroscopy, FTIR, XRD, DLS, EDX and SEM. Assessment of antibacterial activity of biosynthesized ZnO NPs using a well diffusion method revealed the highest zone of inhibition of 28 ± 2 mm (*E. coli*) and 23 ± 3 mm (*S. aureus*) at 100µg/mL concentration. The antioxidant potential of ZnO NPs evaluated using DPPH assay showed the IC₅₀ value of ZnO NPs to be 62.5µg/mL. Cytotoxicity of ZnO NPs on melanoma cell line A375 was evaluated using MTT assay. Overall, this study highlights a promising and sustainable approach for the synthesis of ZnO NPs from biological waste and underscores their potential applications in biomedical fields

Key words: Zinc oxide, nanoparticle, fish waste valorization, biogenic synthesis, biomedical application.

Sustainable Fluorescent Carbon Dot from Marine Waste for Biomedical Applications

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Abstract

Waste valorisation is very important in the sustainable production of valuable chemicals and materials. This study investigates the feasibility of green technology utilising marine waste as a renewable substrate for subsequent carbon dot production through hydrothermal method while evaluating marine waste as a commercial raw material¹. A one-pot hydrothermal method was developed for the green synthesis of highly fluorescent carbon dots (CDs).². The as-synthesized CDs were characterized for its optical properties using UV–Vis, Fluorescence and Fourier transform infrared (FT-IR) spectrophotometry and for structural properties using dynamic light scattering (DLS), X-ray Diffraction (XRD) and field emission Scanning electron microscopy (FE-SEM). The antioxidant capacity of CDs proved to be exceptionally good with good biocompatibility against fibroblast cells. These CDs showed an appreciable zone of inhibition when examined on *E. coli* and *S. aureus* bacterial (gram-positive and gram-negative, respectively) strains at minimum concentrations. Thus, the developed CDs are potential candidates as, antioxidants and antimicrobial agents.

Keywords: Waste valorisation, N-doped carbon dots, Anti-microbial agents

In Vitro Assessment of Nava Rasa Karaisal Against Agricultural Pathogens

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Abstract

The use of synthetic pesticides and antimicrobial agents in agriculture has raised concerns regarding environmental sustainability, residual toxicity and the development of resistant agricultural pathogens. Traditional natural formulations offer a promising alternative for sustainable crop protection. The present study was undertaken to formulate Nava Rasa Karaisal (NRK) and evaluate its in vitro antioxidant, antibacterial, and antifungal activities against selected agricultural pathogens. NRK was prepared using natural components including panchagavya, banana, soil, jaggery and gram flour under controlled fermentation conditions. The antioxidant potential of the formulation was evaluated using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) free-radical scavenging assay. NRK exhibited dose-dependent antioxidant activity, with a maximum scavenging activity of 56.6% at 500 µg/ml and 50.51% at 10 µg/ml, with an IC₅₀ value of 80.29 µg/ml, indicating moderate antioxidant potential. The antibacterial activity was evaluated against *Bacillus cereus* and *Xanthomonas* species using the agar well diffusion method. NRK showed inhibition zones of 8.35 ± 0.21 mm against *B. cereus* and 7.45 ± 0.21 mm against *Xanthomonas* species. Antifungal activity was evaluated against *Fusarium solani*, *Fusarium oxysporum*, *Aspergillus niger* and *Aspergillus ustus*. NRK showed the highest inhibition against *A. niger* (13.55 ± 0.35 mm), followed by *A. ustus* (8.70 ± 0.14 mm) and *F. solani* (7.15 ± 0.07 mm), whereas no inhibition was observed against *F. oxysporum*. NRK combined with pesticide generally showed enhanced antimicrobial activity, whereas combination with antibiotic showed comparatively reduced activity. Overall, the findings demonstrate that NRK possesses measurable antioxidant and broad but selective antimicrobial potential and may serve as a promising natural formulation for sustainable agricultural pathogen management and reduction of dependence on synthetic pesticides.

Keywords: NRK, agricultural pathogens, antimicrobial activity, antioxidant activity, DPPH assay, biocontrol agent; plant pathogens.

Eco-Friendly Synthesis Of (Cu-Zn-Ag) Oxide Nanoparticles Mediated By (*Vanda Testacea*) and Evaluation of Its Antibacterial Activity

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Abstract

In the present study, eco-friendly synthesis of copper-zinc-silver oxide (Cu-Zn-Ag oxide) nanoparticles has been carried out by using extract of *Vanda testacea* as natural reducing and stabilising agent. Green synthesis is an environmentally sustainable alternative to the conventional methods of nanoparticle production, reducing the use of toxic chemicals and hazardous processing conditions. The presence of phytochemicals such as phenolic compounds, flavonoids, alkaloids and other bioactive constituents in *Vanda testacea* might be involved in reducing and stabilising the metal ions during the formation of the nanoparticles. The synthesised nanoparticles will be characterised by suitable analytical techniques such as UV-Vis spectroscopy, FTIR, XRD, SEM and EDX for their optical properties, functional groups, crystalline structure, morphology and elemental composition. The synthesised Cu-Zn-Ag oxide nanoparticles will be subjected to the antibacterial activity against selected Gram-positive and Gram-negative bacterial strains by using suitable microbiological assays. The antibacterial potential of these composites can be attributed to the synergistic effects of copper, zinc, and silver ions, generation of reactive oxygen species, interaction with bacterial cell structures, etc. The present study aims to develop a simple, cost-effective and environment-friendly approach for the synthesis of multifunctional metal oxide nanoparticles having potential applications in antimicrobial and biomedical fields.

Keywords: Antibacterial activity, Antioxidant activity Anticancer activity, *Vanda Testacea*.

Computational Studies on the Structure and Properties of Chemical Compounds Present in Ginger

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Abstract

Nanotechnology and material chemistry are highly inter-related with physics, holds promise and excitement in all areas of science. Ginger is one of the most common spices which contains the main chemical compounds Gingerols, Gingeberene, Gingerone, Shogaol etc., Ginger for many years has been the traditional remedy for colds. Ginger has a sialagogue action, stimulating the production of saliva, which makes swallowing easier. A sialagogue, is a drug or substance that increases the flow rate of saliva. The chemical compounds present in ginger exhibit a host of biological activity, ranging from anticancer, anti-oxidant, anti-microbial, anti-inflammatory and anti-allergic to various central nervous system activities. Material Chemistry and physics can also play an important role in understanding the medicinal efficacy of these molecules. For example, the solubility of these bioactive compounds in water at different temperature were studied using COSMO-RS method and LLE phase diagram was constructed. It concludes that the solubility of these bioactive ginger compounds increases dramatically when the temperature increases from 130- 200 degree. Edible ginger-derived nano-lipids created from a specific population of ginger nanoparticles show promise for effectively targeting and delivering chemotherapeutic drugs used to treat colon cancer which is evidence for future nanomedicine. Though the biological activities of these chemical compounds present in the ginger are known, structural and reactivity studies on these compounds at molecular level are scarce. We have used Density Functional Theory (DFT) computations to explore the structural properties of these molecules at molecular level. The important findings of our work will be presented.

Keywords: Nanotechnology, Ginger, Gingerol, DFT, Bonding, Nanomedicine

Pyrene-Naphthalene Based Schiff Base: Smartphone Integrated Paper-Based Sensor for Copper Sensing and Solid-State Latent Fingerprint Detection

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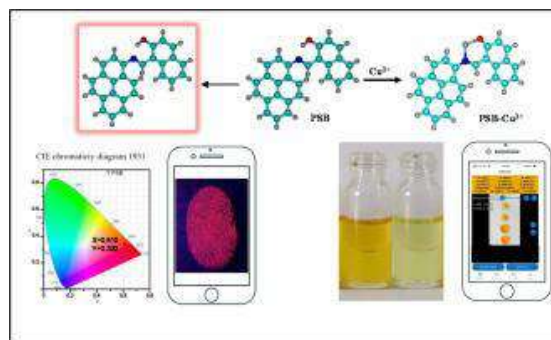
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Abstract

A pyrene-naphthalene based schiff base (PSB) was prepared via the simple condensation between 1- aminopyrene with 2-hydroxy-1-naphthaldehyde and was characterized using FT-IR, NMR, Mass spectrometer and Elemental analysis. The resultant PSB probe was displayed the selective recognition of Cu^{2+} over other competing metal ions and anions in solutionⁱ. The probe underwent a distinct colour change on interacting with Cu^{2+} and the colour change could be visualized with naked eyes. The calculated LODs from absorption titration was found to be $1.7\mu\text{M}$ and the metal-ligand complex was formed at a 1:1 ratio, which was confirmed by Job's plot, and the binding constant was calculated by the Benesi-Hildebrand plot ($5.3 \times 10^4 \text{ M}^{-1}$). A simple analytical platform based on paper substrates and RGB analysis through smart phones was designed to rapidly detect Cu^{2+} ions with a detection limit of $2.28\mu\text{M}$ and showed the potential application to different water samples. In addition, recovery tests were performed on real water samples to establish the potential practical application of this sensor. The red emissive solid state fluorescent probe is capable of visualizing the invisible forensic finger prints thus having an additional advantage of the forensic importance. The newly designed PSB fluorescent probe has the potential of being used for sensing of Cu^{2+} ions due to its inherent sensitivity and specificity, in addition to being a convenient paper-based system and being able to visualize latent fingerprints. This novel sensing platform provides a simple analytical platform which does not require complex instruments in the routine analysis.

Keywords: Schiff base, Metal sensing, Paper-based sensor, RGB detector, Smartphone, Latent fingerprint.



Marine Waste-Derived Nb⁵⁺/Yb³⁺-Modified Hydroxyapatite-Chitosan/Gelatin Composite Coating for Ti-6Al-4V Implants

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Abstract

The development of sustainable multifunctional coatings with improved corrosion resistance and biological performance is highly important for the long-term success of titanium implants. In the present study, a marine biowaste-derived Nb⁵⁺/Yb³⁺-modified hydroxyapatite/chitosan-gelatin (m-HAp/Chn-Gel) composite was developed and deposited onto plasma-treated Ti-6Al-4V substrates using electrophoretic deposition. Hydroxyapatite and chitosan were obtained from crab and prawn shell wastes, respectively, highlighting a sustainable approach for converting marine biowastes into value-added biomaterials. Structural and surface analyses confirmed the formation of a nanocrystalline apatite-based composite coating with successful integration of the chitosan-gelatin matrix. The coating exhibited uniform morphology, nanoscale surface roughness, hydrophilic wettability, enhanced surface hardness, and good thermal stability. Electrochemical investigations demonstrated improved corrosion protection of the Ti-6Al-4V substrate under simulated physiological conditions, with calcium enrichment during immersion contributing to the protective behavior. Biological evaluation using MG-63 osteoblast-like cells revealed concentration-dependent cellular responses while maintaining the nuclear integrity of adherent cells at suitable concentrations. The coating also showed moderate antibacterial activity against *Escherichia coli* and *Staphylococcus epidermidis*. Overall, the developed marine waste-derived m-HAp/Chn-Gel coating demonstrates promising multifunctional characteristics and provides a sustainable surface-engineering strategy for enhancing the corrosion resistance, biological compatibility, and antibacterial performance of Ti-6Al-4V implants.

Keywords: Marine Biowaste; Electrophoretic Deposition; Corrosion Resistance; Antibacterial Activity; Osteoblast Compatibility.

DNA Binding Modes of Carbazole Based Schiff Base Molecule and Molecular Docking of Guanine Quadruplex Structures

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Abstract

This article describes the DNA binding interaction studies of a new carbazole based Schiff base molecule (CS). Electronic absorption, fluorescence spectroscopy, thermal denaturation and viscosity measurements were used to explore the DNA-binding properties of the compound. The results from the DNA melting temperature are in good agreement with the conclusion drawn from absorption titration and viscosity measurements, and suggested that CS could interact with CT-DNA via groove-binding. The Schiff base molecules binding to DNA through intercalation usually results in hypochromism and bathochromism as the intercalation mode involves a strong π - π stacking interaction between an aromatic chromophore and the base pairs of DNA. The extent of the hypochromism in the UV band is consistent with the strength of intercalative interaction. However, a non-intercalative such as groove- and electrostatic-binding modes with DNA may result in hyperchromism deduced from damage to the DNA double-helix structure. A docking study to predict the binding mode of CS to G-quadruplex was performed using ensemble docking. Of the 50 x 5 docking trials, CS resulted in binding to either the loop (22%) or groove regions (78%) of the G-quadruplexes. Our findings indicate that the inclusion of water molecules lead to strong electrostatic effects which are related to the formation of a hydrogen bond network between the aromatic CH=N and OH groups of CS to (a) G-quadruplex backbone (b) to water molecules and (c) between water molecules with other sections of the G-quadruplex, thus result in a total favorable binding energy.

Key words: Fluorescence spectroscopy, Schiff base, Absorption titration, Viscosity measurements, Docking study

Multifunctional Protection of 316L SS Using a Synthetic-Polymer-Free Sm³⁺/Yb³⁺ Co-Doped Hydroxyapatite/Dual-Biopolymer Coating

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Abstract

A multifunctional protective coating was developed for improving the surface performance of 316L stainless steel for biomedical applications. The coating was formulated using Sm³⁺/Yb³⁺ co-doped hydroxyapatite (M-HAP) incorporated into a dual-biopolymer matrix of sodium alginate and κ-Carrageenan (M-HAP/DBP), and was deposited onto plasma-activated 316L stainless steel by electrophoretic deposition. The deposited coating exhibited a thickness of approximately 5.66 μm, with M-HAP particles having an average nanoscale size of ~49.9 nm. The integration of the doped HAP phase with the dual-biopolymer matrix enhanced surface hydrophobicity and micro-Vickers hardness, indicating improved surface durability. Electrochemical measurements in simulated body fluid demonstrated a protection efficiency of 61.57% and a corrosion rate of 0.186 mm year⁻¹. When evaluated in glucose-containing SBF, the coating exhibited an increased protection efficiency of 87.07%, confirming its stable protective response under a modified physiological environment. After 28 days of immersion, only 0.23% mass loss was observed, demonstrating resistance to aqueous degradation. Furthermore, the coating exhibited concentration-dependent antibacterial activity. These findings demonstrate the potential of the synthetic-polymer-free M-HAP/DBP coating as a multifunctional surface for enhancing the durability, corrosion protection, physiological stability, and biological functionality of 316L stainless-steel biomedical implants.

Keywords: Hydroxyapatite; Dual-biopolymer matrix; Electrophoretic deposition; Corrosion protection; Physiological stability; Antibacterial activity

Fluoride Exposure, Dental Fluorosis, and Calcium Depletion: A Pilot Study

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Abstract

Excessive fluoride exposure through drinking water may adversely affect dental health and mineral homeostasis. This pilot cross-sectional study evaluated fluoride exposure, dental abnormalities, and calcium status among healthy adults residing in villages of the Palar River bank belt of the erstwhile Vellore District, Tamil Nadu, India. Participants were screened for eligibility, and relevant demographic, dietary, drinking-water, and medical-history information was collected. Drinking-water, serum, and morning spot urine samples were obtained for fluoride estimation. Dental examination was performed to identify enamel mottling, discoloration, pitting, and other features suggestive of dental fluorosis. Serum calcium, phosphorus, vitamin D, parathyroid hormone, and selected renal-function biomarkers were assessed using established biochemical methods. The relationship between fluoride exposure, dental findings, and calcium status was evaluated using descriptive and correlation analyses. The study aims to characterize fluoride-associated dental changes and investigate whether increased fluoride exposure is accompanied by altered calcium homeostasis among residents of this fluoride-exposed region.

Keywords: Dental fluorosis; Calcium depletion; Calcium homeostasis; Drinking water; Palar River; Vellore District

Anticancer and Anti-inflammatory Properties of Metabolite Derived from Endophyte Bacteria Colonizing Marine *Ulva Lactuca* Seaweed

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Abstract

Human diseases, wounds or infections of any nature are inherently linked with inflammations. Inflammation is linked to many diseases, such as cancer, stroke, and cardiovascular and neurodegenerative disease. At the infection site, microbial proteases can lead to necrosis and apoptosis of phagocytes and cause death of normal tissue cells. Phagocyte dependent growth factors required for cellular proliferation and various healing components are impaired by proteases of infecting microbes and delay wound healing process. Chronic infections are always accompanied by chronic inflammations. The inflammatory signals generated in the host body become the root cause for inducing or severing the tumorigenesis and cancer development in the affected patients. A cost effective un-harmful drug with dual role of anti-inflammatory and anti-bacterial property can be a better therapeutic. The study was focused to marine organisms that have developed unique metabolic abilities to ensure their survival in diverse and hostile habitats. A pan drug resistant VRSA pathogen was employed as challenge pathogen to select an isolate associated with *Ulva lactuca* macroalgae with efficient antimicrobial potency. The screened potential endophytic bacteria *B. subtilis* UEN8 was mass cultured in formulated media under optimized conditions. Bacterial bioactive compounds were extracted, separated, purified and characterized for different biological, chemical and physical methods. In the GC-MS analysis, among the ten numbers of compounds detected in ethyl acetate extract, the 12-methyl-oxa-cyclododecan-2-one in the HPLC purified fraction-2, revealed good bioactivity in dose dependent manner. The toxicity study results indicated its non-cytotoxic nature. Its anti-inflammatory role as confirmed by in-silico studies conferred an advantage for its application in infectious wound managements. The purified bioactive compound of endophyte of marine *Ulva lactuca* alga possessed antimicrobial, antioxidant, QS disrupting and anticancer capability. It can serve a source for drug lead for treating several diseases and infections.

Key words: Chronic infections, Chronic inflammations, *Ulva lactuca* macroalgae, Endophyte, GC-MS, Anti-oxidant, Anti-cancer.

Optimization of Indolyl-Functionalized Chitosan based Hydrogels Using the Taguchi Method for Stimuli-Responsive Swelling

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Abstract

In this study, indolyl-functionalized chitosan-based composite hydrogels were developed and optimized using the Taguchi method to obtain controlled stimuli-responsive swelling behavior. Concentration of Chitosan, indole-2-carboxaldehyde, PVA and crosslinker were selected as four optimization parameters, and an L9 orthogonal array was employed for the experimental design. The synthesized hydrogels were characterized using UV–visible spectroscopy, FTIR spectroscopy, and SEM analysis of the swollen hydrogel morphology. Swelling behavior, biodegradation, solubility, and temperature responsiveness were investigated at 28 and 50 °C. The swelling performance was further evaluated in salt and physiological solutions. The indolyl chitosan–PVA hydrogel exhibited swelling the order glucose > urea > synthetic urine > saline solution. SEM analysis indicated that incorporation of PVA and indole-2-carboxaldehyde into the chitosan matrix increased the surface pore size, contributing to enhanced hydrophilicity and swelling capacity. Overall, the results demonstrate that Taguchi-based formulation optimization provides an effective approach for controlling the swelling characteristics of indolyl-functionalized chitosan-based hydrogels and highlight their potential as stimuli-responsive materials for aqueous and physiological environments.

Keywords: Taguchi method, indole 3-carboxaldehyde, chitosan, hydrogel, stimuli responsive

Investigation of Vanillin-Borate Bioactive Glass/PMMA Composites for New Bone Mineralization, Antibacterial Activity, and Osteoblast Differentiation

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Abstract

Restoring the architecture and biological function of natural bone remains a central challenge in regenerative medicine, and materials that promote bone regeneration while preventing implant-associated infections offer a promising approach to advanced implant design. Borate bioactive glass (BBG) of composition 46.1% B₂O₃, 26.9% CaO, 24.4% Na₂O, and 2.6% P₂O₅ was synthesized by the sol–gel method, and BBG/PMMA and BBG/PMMA/vanillin (VA) composites were fabricated by salt leaching to create porous, bone-mimicking structures. The composites were characterized by FTIR, XRD, and SEM before and after immersion in simulated body fluid (SBF). FTIR confirmed successful composite formation and the XRD revealed a transformation from amorphous glass to crystalline hydroxyapatite (JCPDS 09-0432) after 14 days of SBF immersion, with sharper reflections for BBG/PMMA/VA indicating vanillin-assisted apatite crystallization, while SEM showed mineralization from sparse calcium phosphate nuclei at 3 days to dense apatite layers at 14 days, most pronounced with vanillin. Antimicrobial and antibiofilm activities against *Staphylococcus aureus* and *Escherichia coli* were evaluated by agar well diffusion, broth microdilution (MIC), and biofilm assays, with inhibition zones (50–200 µL) of 12–20 mm for BBG, 14–22 mm for BBG/PMMA, and 15–25 mm for BBG/PMMA/VA, alongside the lowest MIC values and near-complete biofilm suppression (BBG < BBG/PMMA < BBG/PMMA/VA). Cytocompatibility and osteogenic potential were further assessed in MG63 osteoblast-like cells by MTT, Alizarin Red S (ARS), and alkaline phosphatase (ALP) assays. The synergistic integration of PMMA and vanillin thus enhances apatite formation and antimicrobial efficacy, establishing BBG/PMMA/VA as a promising bone tissue engineering candidate with intrinsic protection against implant-associated infections.

Keywords: Bone regeneration, Borate bioactive glass, PMMA, Vanillin.

Recycled Plastic-Based Hybrid Composites for Advanced Body Armor:

A Review

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Abstract

One of the hardest structural polymer composite applications is body armor, which must optimize specific strength, energy absorption, and ballistic-limit velocity within weight and comfort constraints. Para-aramid and ultra-high-molecular-weight polyethylene (UHMWPE) fibers, carbon and glass fibers, and ceramic and metallic strike faces dominate this space and are virtually entirely generated from virgin petrochemical or mining feedstocks. No one offers a reliable end-of-life recycling path. While producing hundreds of millions of tons of plastic garbage annually, less than 20% is recycled into usable products. Our review examines how these issues connect. There is rising technical literature on using recycled thermoplastics, recovered PET, HDPE/LDPE, PP, and associated waste streams as matrices or secondary reinforcements in hybrid composite systems. Exploring how to construct such systems to meet soft and hard body armor performance requirements. Recycling technologies and their effects on polymers, recycled-plastic composite systems reinforced with natural, synthetic, and nanomaterials, and hybridization as the best way to close the performance gap between recycled-content composites and incumb Manufacturing routes, mechanical and ballistic characterization, and material class comparisons are described. After that, the research gaps that separate laboratory-scale recycled-composite studies from a certified, fieldable recycled-content armor product are candidly discussed: recyclate property variability, weak fiber-matrix interfacial bonding, limited high-velocity ballistic test data, and the near-total absence of armor-specific life-cycle and techno-economic studies. The review concludes that recycled-plastic hybrid composites are scientifically credible and environmentally compelling for soft-armor backing layers, trauma-pack liners, training and less-lethal armor, and non-ballistic protective structures, provided that interfacial engineering, recyclate quality control, and standardized ballistic testing protocols mature.

Keywords: recycled plastics; hybrid composites; body armor; ballistic performance; circular economy; fiber reinforcement; sustainable materials

Lead, Iron, and Zinc in Male Reproductive Health: A Narrative Review

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Abstract

Male infertility is an increasing global health concern, with trace elements and toxic metals influencing reproductive physiology. This narrative review synthesizes evidence on lead (Pb), iron (Fe), and zinc (Zn), focusing on trace-element homeostasis, exposure-related reproductive outcomes, and molecular mechanisms. Literature published between January 2000 and December 2025 was identified through PubMed, Scopus, and Web of Science. Relevant human clinical and epidemiological studies were prioritized, while selected animal and in vitro studies supported mechanistic interpretation. Lead exposure was associated with impaired sperm motility, abnormal morphology, increased DNA fragmentation, and endocrine disruption. Iron exhibited concentration-dependent effects, supporting mitochondrial function and spermatogenesis at physiological levels but promoting oxidative stress and hormonal imbalance when dysregulated. Zinc contributed to sperm chromatin stabilization, testosterone biosynthesis, and sperm maturation; deficiency was linked to reduced semen quality and reproductive potential. Maintaining trace-element balance, optimizing zinc and iron status, and minimizing lead exposure may support male reproductive health.

Keywords: Male fertility; Zinc; Lead; Iron; Spermatogenesis; Semen quality; Oxidative stress.

Dental Point Net: A Multi-Head Deep Learning Architecture for Automated Classification of Dental Arch Status Using Three-Dimensional Intraoral Data

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Abstract

Accurate Kennedy classification of the partially edentulous dental arch underpins removable partial denture (RPD) design, yet conventional classification relies on subjective clinical assessment, introducing inter-examiner variability and creating a workflow discontinuity with three-dimensional (3D) digital prosthodontic pipelines. We present DentalPointNet, a multihead deep learning architecture that operates directly on 3D point-cloud data derived from intraoral scanner (IOS) STL files to simultaneously classify Kennedy class (I–IV), arch identity (maxillary/mandibular), and modification-space count (0–3). The system forms the AI classification engine of a patented integrated hardware–software healthcare platform (Indian Patent Application No. 202641094644; Copyright No. SW-23665/2025-CO) incorporating a novel unified dental arch classification nomenclature that generates machine-readable hierarchical diagnostic codes directly compatible with digital laboratory workflows. A dataset of 562 IOS-derived point clouds from 112 patients, partitioned by patient into training, validation and test sets, was used to evaluate three architectural configurations. The final validated configuration — a PointNet++ single-scale-grouping (SSG) backbone with classbalanced sampling, focal loss and test-time augmentation — achieved 80.0% Kennedy-class accuracy (macro-F1: 77.0%), 98.9% arch accuracy (macro-F1: 98.8%), and 90.0% modification-space accuracy on the held-out test set, substantially exceeding majority-class baselines across all outputs. These findings establish the technical feasibility of automated, geometry-native Kennedy classification as an enabling component of AI-assisted digital RPD design workflows.

Synthesis and Characterization of Liposomal Encapsulated Particles for Enhanced Therapeutic Efficiency in L929 Cell Lines

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Abstract

Medicinal plants are important sources of bioactive compounds with potential applications in the prevention and management of various diseases. *Gymnema sylvestre*, commonly known as “Gurmar” or the “sugar destroyer,” is a woody climbing plant traditionally used in Indian medicine for its antidiabetic properties, particularly its ability to help regulate blood glucose levels and suppress the perception of sweet taste. Gymnemic acid, a major bioactive constituent of *G. sylvestre*, has demonstrated promising therapeutic potential; however, its effective delivery may be limited by its physicochemical and bioavailability characteristics. The present study aims to develop a lipid-based carrier system for the encapsulation and delivery of gymnemic acid to enhance its therapeutic efficacy and improve its delivery characteristics. Gymnemic acid will be incorporated into the lipid-based carrier, and the developed formulation will be evaluated for its physicochemical properties and drug-loading efficiency. Qualitative and quantitative estimation of gymnemic acid will be performed using suitable analytical methods, including UV–Visible spectrophotometry. The optimized formulation will be characterized using Fourier-transform infrared spectroscopy (FTIR), particle size, polydispersity index (PDI), and zeta potential measurements to investigate drug–carrier interactions, functional groups, particle-size distribution, surface charge, and formulation stability. Furthermore, the optimized formulation will be evaluated *in vitro* using the L929 cell line to determine its cellular compatibility and preliminary therapeutic potential. Overall, the study is expected to provide a promising lipid-based delivery approach for gymnemic acid and may contribute to the development of a safer, efficient, and more targeted system for its therapeutic application.

Keywords: Gymnemic acid, Lipid based carrier, Encapsulation, Therapeutic efficiency.

Cadmium-Induced Reproductive Toxicity in Male Rats: An In Vivo Study

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Abstract

Cadmium is an environmental toxicant that can adversely affect testicular function through oxidative stress, endocrine disruption, and cellular damage. This in vivo study investigated the effects of cadmium exposure on reproductive function in male rats. Young male Wistar rats were exposed to cadmium chloride at a dose of 1.1 mg/kg body weight/day for 48 days. Reproductive toxicity was evaluated by assessing body and testicular weights, sperm concentration, motility, morphology, and viability. Serum testosterone and selected biochemical markers, including electrolytes and oxidative DNA damage indicators, were also measured. Testicular tissue alterations were assessed using histopathological examination. Cadmium exposure was associated with progressive changes in body weight, testicular atrophy, impaired sperm quality, altered testosterone levels, and disturbances in mineral homeostasis. Increased oxidative DNA damage was also observed, suggesting that oxidative stress contributes to cadmium-induced reproductive dysfunction. These findings demonstrate that prolonged cadmium exposure adversely affects male reproductive health and may compromise fertility through combined testicular, endocrine, and oxidative mechanisms.

Keywords: Cadmium; Male fertility; Wistar rats; Testicular toxicity; Sperm quality; Testosterone; Oxidative stress; Reproductive toxicity.

Metal Toxicity and Diabetes Risk in Vellore District: A Pilot Study

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Abstract

Exposure to toxic metals through contaminated drinking water may contribute to metabolic disturbances associated with diabetes mellitus. This pilot cross-sectional study aims to investigate the association between lead and arsenic exposure and diabetes-related biomarkers among adults residing in selected villages of Vellore District, Tamil Nadu, India. Participants will be screened for demographic characteristics, dietary habits, drinking-water sources, family history of diabetes, and relevant medical conditions. Drinking-water, blood, and morning spot urine samples will be collected for estimation of lead, arsenic, and selected biochemical parameters. Glycemic status will be assessed using fasting blood glucose, postprandial blood glucose, glycated haemoglobin, and serum insulin, where applicable. Additional biomarkers of renal function and oxidative stress will be evaluated to explore potential mechanisms linking metal exposure with metabolic dysfunction. Descriptive, correlation, and regression analyses will be performed to assess relationships between metal concentrations and diabetes-related parameters. The findings may provide preliminary evidence regarding metal-associated metabolic alterations and diabetes risk in this population.

Keywords

Lead; Arsenic; Metal toxicity; Diabetes mellitus; Glycemic control; Insulin resistance; Fasting blood glucose; HbA1c; Vellore District; Pilot study.

Metal Toxicity, Stress, and Obesity: A Primary Study

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Abstract

Exposure to toxic metals may contribute to obesity-related metabolic disturbances through oxidative stress, inflammation, and altered endocrine regulation. This primary cross-sectional study investigated the association between lead and arsenic exposure, stress-related biomarkers, and obesity among adults residing in selected villages of Vellore District, Tamil Nadu, India. Participants were evaluated using demographic, dietary, lifestyle, and anthropometric assessments. Body mass index, waist circumference, and other obesity-related parameters were recorded. Drinking-water, blood, and morning spot urine samples were collected for estimation of lead, arsenic, and selected biochemical biomarkers. Stress-related alterations were assessed using appropriate biochemical and/or validated psychological measures. Metabolic status was evaluated using fasting blood glucose, lipid profile, insulin-related parameters, and selected oxidative stress biomarkers. Descriptive, correlation, and regression analyses were performed to determine relationships between metal exposure, stress, and obesity-related outcomes. The study may provide preliminary evidence regarding the potential contribution of toxic-metal exposure and stress-associated metabolic alterations to obesity in this population.

Keywords: Lead; Arsenic; Stress; Obesity; Oxidative stress; Metabolic dysfunction; Body mass index

Bimetallic Nanoparticle Incorporated biopatches for promoting antibacterial and diabetic wound dressings

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Abstract

Restoring diabetic wounds requires dynamic control of the pathological wound microenvironment in concert with tissue regeneration a complex therapeutic challenge arising from the persistent imbalance in cellular, biochemical and inflammatory processes. To address these challenges, we here in propose to use the biomimetic curcumin-incorporated chitosan gelatin (CGC) Biopatch reinforced with bimetallic Fe-Co nanoparticles was developed for enhanced wound healing. Two distinct metallo- biopatch formulations were fabricated, namely CGC-Fe/CO-NL metallo-biopatch (where NL-non-crosslinked) and CGC-Fe/CO-XL metallobiopatch (where XL-guteraldehyde crosslinked) and comprehensively characterized to elucidate their physicochemical and functional properties. FTIR analysis confirmed strong intermolecular interactions between the polymer matrix and drug, while XRD analysis indicated a predominantly amorphous structure conducive to uniform bioactive component distribution. SEM analysis demonstrated that crosslinking CGC-Fe/CO-XL produced a smoother and more compact surface with homogeneously distributed nanoparticles, in contrast the non-crosslinked CGC-Fe/CO-NL bipatch exhibited a relatively rough and porous surface. Enhanced thermal stability was also observed following crosslinking. The optimized CGCFe/Co-XL biopatch exhibited antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*, producing inhibition zone of 10 and 12 mm, along with $85.4 \pm 2.1\%$ at DPPH radical -scavenging activity at 50 $\mu\text{g/mL}$ and improved hemocompatibility. In addition, fibroblast viability exceeds 90% the material promoted cell migration, resulting in near complete wound closure, within 24h. These findings establish the CGC-Fe/Co-XL metallo biopatch as a multifunctional biomaterial with strong potential for diabetic wound dressing applications.

Key words: Chitosan-gelatin biopatch, Curcumin, Fe-Co nanoparticles, Crosslinked biopatch, Diabetic wound healing.

Nano-Cellulose Based Hemostatic Patch from Banana Peel

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Abstract

Uncontrolled bleeding resulting from injuries, wounds, accidents, and surgical procedures is a significant clinical concern that requires rapid and effective intervention to prevent excessive blood loss and associated complications. Conventional hemostatic materials are available for bleeding control; however, their cost, limited biodegradability, and dependence on synthetic or non-renewable materials have created a need for sustainable, biocompatible, and economically viable alternatives. In this context, agricultural waste materials containing naturally occurring polymers offer considerable potential for the development of value-added biomedical products. The present project focuses on the development of a nanocellulose-based hemostatic patch derived from banana peel, an abundantly available and biodegradable agricultural residue. Banana peel contains a considerable amount of cellulose, which can be isolated through suitable chemical treatment and subsequently processed into nanocellulose. At the nanoscale, cellulose exhibits a high surface-area-to-volume ratio and enhanced surface characteristics, making it a promising material for biomedical applications. The extracted nanocellulose is proposed to be incorporated into a suitable patch formulation to obtain a flexible, lightweight, absorbent, and biocompatible wound dressing. The developed patch is intended to facilitate rapid blood absorption at the wound site and promote the concentration and interaction of blood components, thereby supporting the natural coagulation process and accelerating clot formation. The fabricated nanocellulose-based patch can be systematically evaluated to determine its suitability for hemostatic applications. Important physicochemical and functional properties, including water absorption capacity, swelling behaviour, surface morphology, mechanical strength, biodegradability, and stability, can be investigated. Its hemostatic performance can be assessed through appropriate blood-clotting and coagulation-related studies. In addition, antibacterial activity and biocompatibility evaluations can be performed to determine its potential for safe wound management and to minimize the risk of infection and adverse biological responses. The proposed approach provides an environmentally responsible method for utilizing banana peel waste and converting it into a functional biomedical material. This not only contributes to waste reduction and sustainable material development but also promotes the concept of a circular bioeconomy by transforming an agricultural by-product into a value-added healthcare product. The developed patch may have potential applications in first-aid wound care, minor cuts and injuries, trauma management, and supportive bleeding control during medical procedures. Overall, the project aims to establish banana-peel-derived nanocellulose as a promising, sustainable, and cost-effective material for the development of next-generation hemostatic wound dressings.

Keywords: Nanocellulose, Banana Peel, Hemostatic Patch, Wound Dressing, Hemostasis.

Enhanced Cytotoxic activity of Zinc oxide Nanoparticles of *Corallocarpus epigaeus* against TPC-1 Human Papillary Thyroid Carcinoma Cell Line

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Abstract

Papillary thyroid carcinoma is the most common type of thyroid malignancy, and the development of effective and safer therapeutic approaches remains an important area of cancer research. Plant-mediated synthesis of nanoparticles has gained considerable attention because phytochemicals may contribute to nanoparticle formation and enhance their biological activities. *Corallocarpus epigaeus*, a medicinal plant traditionally used in South Indian medicine, contains diverse bioactive phytoconstituents with potential therapeutic properties. The present study aimed to synthesize zinc oxide nanoparticles (ZnO-NPs) using *Corallocarpus epigaeus* extract and evaluate their cytotoxic activity against the TPC-1 human papillary thyroid carcinoma cell line. *C. epigaeus*-mediated ZnO-NPs were synthesized using a green synthesis approach and characterized using appropriate physicochemical techniques. The cytotoxic effect of the synthesized nanoparticles on TPC-1 cells was evaluated using an in-vitro cell viability assay at different concentrations. The percentage of cell viability and inhibition was determined, and the concentration producing 50% inhibition of cell viability (IC₅₀) was estimated. Morphological changes in treated cells were also assessed and compared with untreated control cells. Treatment with *C. epigaeus*-mediated ZnO-NPs produced a concentration-dependent reduction in TPC-1 cell viability. Increasing nanoparticle concentrations resulted in progressive morphological alterations and loss of viable cells compared with untreated controls. The observed cytotoxic response indicates the potential of the synthesized ZnO-NPs as a candidate for further investigation against papillary thyroid carcinoma. The findings suggest that *C. epigaeus*-mediated ZnO-NPs possess promising in-vitro cytotoxic activity against TPC-1 cells. Further studies focusing on oxidative stress, apoptosis, molecular mechanisms, and in-vivo efficacy are warranted to establish their therapeutic potential.

Keywords: *Corollocarpus epigaeus*, ZnO nanoparticles, MTT assay, TPC-1, Thyroid cancer

To Compare the Cost-Effectiveness and Safety of Timolol Maleate and Latanoprost in Patients with Glaucoma in Tertiary Care Hospital

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Abstract

In the world of eye diseases, Glaucoma is a serious chronic ocular condition that causes irreversible visual disability if left untreated can lead to sight loss. Treatment options include various medications. Evaluation of the clinical outcomes along with pharmacoeconomic analysis offering valuable treatment approaches. This study aimed to investigate the cost-effectiveness and safety of latanoprost against timolol maleate in glaucoma patients, A prospective observational study was conducted on 100 patients in the ophthalmology department of a tertiary care hospital in Salem from Jan to June 2024. Out of 100 patients, 50 received latanoprost meanwhile 50 patients received timolol maleate. The patients were interviewed using a comprehensive questionnaire to collect the various demographic characteristics and IOP measurements, Visual acuity (VA) and Visual field (HFA) were evaluated. The patients were reviewed after 2nd, 4th, 8th, and 12th weeks for cure rate and cost-utilization. The outcomes were statistically analyzed and were presented in the form of percentages. Although Clinical data revealed at the end of 12 weeks, latanoprost 0.005% shows dominance in its efficacy (36.0 % decrease in IOP from baseline) while Timolol maleate 0.5% had a reduction in IOP by 35.0%. Visual acuity, cup: disc ratio and HFA evaluation show both treatments were safe. In view of Cost-effectiveness, timolol maleate was lower than latanoprost. So, it would be preferable to initiate treatment with timolol maleate. This research concluded that it encourages the physician to cautiously consider while selecting the treatment options as well as regimens depending upon the patient's clinical needs and budgetary expectations.

Keywords: Glaucoma, Intraocular pressure, Visual acuity, Latanoprost, Timolol maleate, cost-effectiveness

In Silico ADME Properties of Carotenoids of Corn Seed

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Abstract

Corn (*Zea mays*) seeds are a rich source of bioactive phytochemicals, including carotenoids such as lutein and zeaxanthin, which are associated with eye health and antioxidant activity. Despite their traditional and nutritional relevance, the pharmacokinetic behaviour of these compounds remains poorly characterized. In this study, the absorption, distribution, metabolism, and excretion (ADME) properties of eight carotenoids from corn seed — lutein, cyclosadol, β -cryptoxanthin, zeaxanthin, α -carotene, β -carotene, α -cryptoxanthin, and β -cryptoxanthin — were evaluated using the SwissADME web tool. Physicochemical properties, lipophilicity, water solubility, pharmacokinetic parameters, drug-likeness (Lipinski, Ghose, Veber, Egan, and Muegge rules), bioavailability scores, and BOILED-Egg predictions were computed for each compound. Results showed that compounds 2–8 violated the Lipinski rule of five (primarily due to high lipophilicity, $MLOGP > 4.15$), while lutein (compound 1) did not exhibit a computable drug-likeness or bioavailability profile. Bioavailability radar analysis indicated that saturation and polarity parameters for all compounds fell within recommended ranges, while size, lipophilicity, and insolubility parameters largely fell outside optimal bounds. The BOILED-Egg model revealed that all eight carotenoids lay outside the white region, indicating negligible passive gastrointestinal absorption and blood-brain barrier permeation. These findings suggest that despite their reported health benefits, corn seed carotenoids possess poor oral bioavailability profiles under standard in silico prediction models, highlighting the need for formulation strategies (e.g., nanoencapsulation) to enhance their pharmacokinetic performance. This study provides baseline computational data to guide future experimental and drug-delivery research on corn-derived carotenoids.

Keywords: Corn seed, carotenoids, in silico ADME, SwissADME, drug-likeness, bioavailability, BOILED-Egg model

Biopolymer Based Composite – A Promising Treasure

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Abstract

World is becoming attracted to the production of novel materials, made primarily of polymers because of their advantages and key roles, in the circular economy concept and model. Unfortunately, the use of plastic-based materials and consumer's preferences for non-biodegradable materials is becoming a serious concern for environmental experts. Utilization of synthetic fiber-reinforced composites is extensive due to their promising strength, flexibility and rigidity. Despite its advantages, decomposition of these materials leads to the emission of hazardous leachate and gases. Environmental concerns and plastic waste generation have led human beings to reconsider the consumption of plastics owing to deleterious effect to the environmental pollution. To sidestep these drawbacks, synthetic fibers and polymers have been replaced with biopolymers and biocomposites. Biopolymers are natural polymers derived from renewable sources such as plants, algae, and microbes. Biopolymers are gaining huge applications in the dental field with the application of scaffolds, Bio-membranes and Nano-composites due to their versatile nature, flexibility and their characteristic nature of binding with monomers. These biopolymers are found to contribute significantly in lowering the carbon footprint compared to conventional plastics. It is also found that blending of nanoparticles and antibiotics with biopolymers has resulted in antimicrobial, antioxidant and anti-inflammatory properties. Bio-composites with excellent durability, performance, and reliability must be produced to broaden their applications. As scientific breakthroughs and technologies advance fresh areas of applications of natural fiber-reinforced composites will emerge, influencing the always-expanding market for bio-based composites.

**A Comparative Study on Drug Utilization Pattern and Cost-Effectiveness
Analysis of Ciprofloxacin, Moxifloxacin, Ciprofloxacin with
Dexamethasone and Moxifloxacin with Dexamethasone Eye Drops in
Bacterial Conjunctivitis**

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Abstract

Bacterial conjunctivitis is a common ocular infection characterized by conjunctival redness, discharge, irritation, and inflammation. This study aimed to compare the drug utilization pattern and cost-effectiveness of ciprofloxacin, moxifloxacin, ciprofloxacin with dexamethasone, and moxifloxacin with dexamethasone eye drops in patients with bacterial conjunctivitis. A six-month prospective observational study was conducted in the ophthalmology department of a tertiary care hospital in Salem. A total of 120 patients were included. Data concerning demographic characteristics, clinical findings, prescribed medications, treatment outcomes, adverse effects, treatment costs, and quality-of-life outcomes were collected and analyzed. Moxifloxacin was the most frequently utilized medication (54.2%), followed by ciprofloxacin (19.2%), moxifloxacin with dexamethasone (15.0%), and ciprofloxacin with dexamethasone (11.7%). Males accounted for 58% of the study population, while females accounted for 42%. The 16–30-year age group showed the highest occurrence (30.83%). Conjunctival hyperaemia was observed in all patients, whereas purulent discharge was reported in 78.3%. The moxifloxacin with dexamethasone group demonstrated a mean recovery time of 5.8 ± 1.1 days, compared with 6.9 ± 1.6 days for the ciprofloxacin group. Ciprofloxacin had the lowest treatment cost and cost-effectiveness ratio, whereas moxifloxacin-based therapy showed higher QALY outcomes. The findings demonstrate differences in clinical recovery, cost, and quality-of-life outcomes, supporting individualized treatment selection based on clinical condition, safety, affordability, and patient requirements. These results may help clinicians balance therapeutic effectiveness, economic burden, safety monitoring, and patient-centered outcomes during routine ophthalmic management and follow-up.

Keywords: Bacterial conjunctivitis, Ciprofloxacin, Moxifloxacin, Dexamethasone, Drug utilization, Cost-effectiveness analysis, QALY, Eye drops.

Hormonal Imbalances and Stress-Mediated Mechanisms Influencing Female Fertility

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Abstract

Female reproductive function is regulated by a complex interaction between the hypothalamic–pituitary–ovarian (HPO) axis, metabolic homeostasis and cellular stress responses. Disruption of hormonal equilibrium can interfere with follicular development, ovulation, oocyte quality and endometrial receptivity, thereby contributing to impaired fertility. Chronic physiological and environmental stress may further influence reproductive function through activation of the hypothalamic–pituitary–adrenal axis and altered glucocorticoid signalling. Increased oxidative stress and associated inflammatory responses may adversely affect ovarian steroidogenesis, mitochondrial function and cellular integrity. Alterations in key reproductive hormones, including gonadotropins, estrogen, progesterone, anti-Müllerian hormone and stress-associated cortisol, may therefore represent important indicators of disturbed reproductive homeostasis. The interaction between endocrine imbalance, oxidative stress and inflammatory signalling may create a mechanistic link between environmental or physiological stressors and female reproductive dysfunction. Understanding these interconnected pathways is important for identifying potential biomarkers and developing preventive and therapeutic strategies for fertility management. A systems-level approach integrating hormonal, oxidative-stress, metabolic and reproductive parameters may provide better insight into the multifactorial mechanisms underlying female infertility.

Keywords: Female fertility; Hormonal imbalance; HPO axis; Oxidative stress; Cortisol; Estrogen; Progesterone; Ovarian function; Reproductive health; Stress mechanisms.

OP-BM-75

Phytochemical, Agricultural, and Eco-Health Dimensions of Germinated Grains (Mulaippari) in Traditional Tamil Practices: Implications for Bio-Nanoscience and Agri-Health

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Abstract

Mulaippari is a traditional women-centered ritual in Tamil Nadu involving the dark-germination of *Navadhanyam* (nine types of grains and pulses) in earthen pots during village festivals. While historically evaluated through anthropological and devotional frameworks, the underlying plant physiology and biochemical transformations during this structured 9-day germination process hold significant relevance for modern agricultural biotechnology and green nanoscience. Germination induces significant metabolic changes in sprouted grains, leading to the synthesis of bioactive phytochemicals (polyphenols, flavonoids, and essential amino acids) and enzymatic activations that enhance seed vigor and stress tolerance. From a bio-nanoscience perspective, these phytochemical-rich sprout extracts serve as natural reducing, capping, and stabilizing agents for the eco-friendly green synthesis of metallic and metal-oxide nanoparticles (e.g., Ag, ZnO, TiO₂) without toxic chemical reagents. Furthermore, the practice functions as an indigenous seed-viability and germination-capacity test for traditional crop varieties prior to the agricultural season. Integrating the biochemical evaluation of *Mulaippari* sprouts with nanotechnology offers promising avenues for developing nano-biofertilizers, eco-friendly crop protection agents, and sustainable agri-health solutions, bridging ancient agro-cultural wisdom with contemporary bio-nanotechnology.

Keywords: Mulaippari; Navadhanyam; Phytochemicals; Green Synthesis; Nanotechnology in Agriculture; Eco-Health.

In Silico Network Pharmacology and Molecular Docking of Kigelia Africana compounds against Acquired Generalised Lipodystrophy (AGL)

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Abstract

Acquired generalized lipodystrophy is a rare lipodystrophy syndrome. It is characterized by selective loss of adipose tissue and is a syndrome of insulin resistance. The study focuses on the important biological features such as the loss of adipose tissue, abnormal lipid metabolism, insulin resistance and metabolic abnormalities. Kigelia Africana phytochemicals drug likeness and interaction in pathways were obtained from referencing articles and were finalized as follows: verminoside, verbascoside, specioside, minecoside, caffeic acid, p-coumaric acid, ferulic acid. The disease target network was retrieved from Genecards database with 3 search terms with filter protein coding and adipose tissue: "Acquired generalized lipodystrophy", "generalized lipodystrophy", "Lipodystrophy insulin resistance". Based on relevance score from 100 initial compounds were narrowed to 10 for constructing drug target network. STRING platform was used for KEGG analysis identifying vital pathways involved. Autodock vina a virtual screening tool was used in docking the identified master hub genes: EGFR and PPARG against phytochemicals. This revealed favorable binding affinities that confirming that Kigelia Africana has therapeutic potential for treating the syndrome. Thus, the results give strong foundation for downstream analysis of bioactive components against key pathways establishing justification for validation of biomedical applications.

Keywords: Acquired generalised lipodystrophy, Kigelia africana, Network pharmacology, Enrichment analysis

Picosecond Laser-Induced Micro–Nano Surface Texturing of Ti6Al4V for Enhanced Implant Surface Characteristics

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Abstract

Laser surface texturing is an effective approach to enhance the surface characteristics of Ti6Al4V towards biomedical implant applications. In the present study, Ti6Al4V surfaces were laser textured to develop hierarchical micro–nano surface features. Their morphological, physicochemical, crystalline and electrochemical characteristics were investigated. Scanning electron microscopy revealed the formation of distinct microscale textures decorated with nanoscale features following laser treatment. Compared with pristine Ti6Al4V, the laser-textured surfaces exhibited increased surface roughness and surface energy, accompanied by improved hydrophilicity. Among the investigated surfaces, the sample with line-dominated features showed the highest surface roughness and wettability. Overall, the combination of hierarchical micro–nano morphology, increased roughness, enhanced surface energy and improved hydrophilicity demonstrate the potential of laser texturing for favorable biological surface interactions and bone–implant integration. These characteristics indicate enhanced interaction with physiological fluids and suggest that laser-textured Ti6Al4V, has potential for bone–implant integration. The laser-induced surface modifications were associated with changes in the overall surface architecture, which can influence the interaction between the implant and the surrounding biological environment. The development of multiscale features provides additional surface area and may influence the adsorption of proteins and other biological molecules at the interface. Controlled modification of surface topography offers a promising way for modifying implant surfaces without altering the bulk properties of Ti6Al4V. The observed changes highlight the importance of laser processing for producing functionalized metallic surfaces. Thus, picosecond laser texturing provides a versatile strategy for developing Ti6Al4V with characteristics suitable for advanced biomedical applications.

Keywords: Laser surface texturing, Ti6Al4V, Hierarchical micro–nano structures, Electrochemical corrosion.

OP-BM-78

Synthesis, Characterization and Antibacterial activity of Schiff base ligand N'-((2 hydroxynaphthalen-1-yl) methylene) hydrazinethiocarbohydrazide

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Abstract

A Schiff base ligand was synthesized through the condensation of 2-hydroxy-1-naphthaldehyde with thiocarbohydrazide in dry methanol under reflux conditions for six hours, yielding a yellow crystalline compound with 87% yield and a melting point of 170 °C. The ligand was characterized using spectroscopic techniques including FT-IR (Jasco FT-IR-4100, 400-4000 cm⁻¹) and ¹H NMR (Bruker 400 MHz, DMSO, TMS as reference). The spectral data confirmed the formation of the desired Schiff base. The antimicrobial activity of the synthesized ligand was evaluated using the agar well diffusion method against selected microorganisms. Different concentrations (20 µl, 40 µl, and 60 µl) of the compound were tested, and the zones of inhibition were measured after incubation at 37 °C for 24 hours. The results revealed significant antimicrobial activity, which increased proportionally with concentration, indicating the potential of the synthesized ligand as an effective antimicrobial agent.

Keywords: Synthesis, Characterization, Antioxidant.

Clinical, Nutritional and Lifestyle Determinants of Osteoporotic Fracture Risk in Postmenopausal Women: A Systematic Review

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Abstract

Postmenopausal women have high fragility fracture and osteoporotic risk due to decrease in oestrogen levels and bone loss related to age. Fracture risk is influenced by many clinical, nutritional and lifestyle factors but their contributions differ across population. A systematic literature review was conducted in PUBMED, Scopus and Web of Science for the literatures published between 2017 January to 2026 September. Determinants of Clinical, nutritional and lifestyle evaluating studies were included. Data on characteristics of study, determinants, fracture outcomes and association measurement were taken. Methodological quality was assessed using appropriate risk-of-bias tools, and results were synthesized quantitatively where suitable. The risk of osteoporotic fracture is influenced by various interacting determinants. Older age, previous fracture, low BMI, prolonged postmenopausal duration, reduced bone mineral density and comorbidities were associated with increased risk of fracture. Recent study showed hypertension, diabetes, alcohol consumption and reproductive characters are the main factors that have risk of fracture. Obesity shows modest risk and nutritional factors like mainly calcium and vitamin D showed strong association in various studies, physical activity and increased fall risk were also associated with increased risk outcomes. Overall, the evidence supports a multidimensional rather than single-factor approach to fracture-risk assessment. Combination of clinical, nutritional and lifestyle factors determine the risk of osteoporotic fracture in postmenopausal women. Integrating modifiable determinants with established clinical risk factors may improve early detection of women at high risk of fracture and encourage individualised preventive strategies.

Keywords: Postmenopausal women, Osteoporosis, Osteoporotic fracture, Fracture risk, Clinical determinants, Nutritional factors.

Role Of Homoeopathy in Conduct Disorder:

A Scoping Review

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Abstract

Conduct Disorder (CD) is a repetitive rule breaking, aggressive and disregard for others condition. It is categorized under severe externalizing psychiatric conditions of childhood and adolescence. Homoeopathy is an individualized treatment method that has a potential role in children and adolescent psychiatry (CAP). However, there is a lack of synthesized mapping of the evidence in the role of Homeopathy in conduct disorder. A systematic approach to map evidence on the role of homeopathy by using clinical research published in the peer reviewed journals between the last two decades, 2005 and 2025. Two electronic database searches were conducted across PubMed/MEDLINE and Google Scholar using Keywords are “conduct disorder”, “oppositional defiant disorder”, “disruptive behavioural disorder”, “childhood aggression”, and “homoeopathy”. The collected information has been collated, summarized, and the results are presented in tables and charts. In total, nine primary clinical studies were included; four multi-case series, two observational studies and three structured case reports. Individualized Homoeopathic medicines that showed favourable outcomes were Anacardium orientale, Belladonna, Chamomilla, Hyoscyamus niger, Nux vomica, Stramonium, Tarentula hispanica, and quantitative outcome measures reported were decreases in Conduct Disorder Rating Scale (CDRS), Disruptive Behavior Disorders Rating Scale (DBDRS), and Vanderbilt ADHD and Disruptive Behavior Diagnostic Parent Rating Scale (VADPRS). Evidence in the literature suggests that individualized homoeopathic treatment reduces disruptive symptoms and emotional dysregulation in conduct disorder. However, further research including well designed randomized controlled trials are warranted to strengthen the evidence.

Keywords: Childhood And Adolescent psychiatry (CAP), Conduct disorder (CD), Homoeopathy, Scoping review.

Green Synthesis and Characterization of Solanum Trilobatum-Mediated ZnO Nanoparticles and Evaluation of Their Antibacterial Activity Against Multidrug-Resistant Bacteria

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Abstract

The present study focuses on the green synthesis of zinc oxide nanoparticles (ZnO-NPs) using an aqueous extract of *Solanum trilobatum*, a medicinal plant traditionally recognized for its diverse pharmacological properties. The phytochemicals present in the plant extract act as natural reducing, stabilizing, and capping agents during the formation of ZnO nanoparticles, providing an environmentally friendly alternative to conventional chemical synthesis methods. The synthesized ZnO-NPs will be characterized using ultraviolet-visible (UV-Vis) spectroscopy, Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and thermogravimetric analysis (TGA), where applicable. These techniques will be used to determine the optical properties, functional groups, crystalline structure, morphology, particle size, and thermal stability of the synthesized nanoparticles. The biological activity of the ZnO-NPs will be evaluated, particularly their antibacterial activity against selected bacterial strains. The antibacterial properties may be associated with nanoparticle–cell membrane interactions, generation of reactive oxygen species, and release of zinc ions. The study aims to demonstrate the potential of *Solanum trilobatum*-mediated ZnO nanoparticles as eco-friendly nanomaterials with promising applications in biomedical and antimicrobial research. *Solanum trilobatum* contains various bioactive constituents, including alkaloids, flavonoids, phenolic compounds, saponins, tannins, terpenoids, and other secondary metabolites. These compounds can participate in the formation and stabilization of ZnO nanoparticles.

A Comparative Cross-Sectional Study on Knowledge, Attitude and Practice Towards Over-The-Counter Medication Among Urban and Rural Populations

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Abstract

Over-the-counter (OTC) medicines are commonly used for managing minor health problems because they are easily accessible and convenient to obtain without a prescription. However, inappropriate self-medication can result in adverse drug reactions, drug interactions, incorrect dosing, and delayed medical consultation. This study assessed and compared knowledge, attitude, and practice regarding OTC medication among rural and urban populations in Salem district. A prospective observational cross-sectional study was conducted among 130 participants aged 18 years and above. Among the participants, 52% were from rural areas and 48% from urban areas. Fever was the most frequently reported condition for OTC medicine use (45%), followed by headache (22%), cold or flu (12%), and pain (10%). Painkillers were among the most commonly used OTC medicines, particularly for immediate symptom relief. The major reason for self-medication was the perception of having a simple illness (50%), followed by the need for quick relief (21%). Pharmacists were the principal source of information about OTC medicines (48%), followed by family and friends (27%) and previous prescriptions (13%). Most participants reported using OTC medicines rarely (60%), while 32% used them occasionally and 8% frequently. Safe-use practices were also observed, with 78.3% reporting that they read medicine labels and 82.5% checking expiry dates before use. Despite satisfactory knowledge and generally positive attitudes towards OTC medicines, 63.3% reported using them without consulting a doctor. These findings highlight the importance of pharmacist counselling, patient education, and community awareness to encourage rational and responsible use of OTC medicines and reduce the risks associated with inappropriate self-medication.

Key Words: OTC Medication, Knowledge, Painkillers, Drug Interaction, Adverse drug reaction, pharmacist.

Impact of Chloride on the Corrosion Behavior of Pure Titanium & Titanium Alloy Coupled with Gold Alloy & Nickel-Chromium Alloy

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Abstract

Titanium and Titanium alloy (Ti6Al4V) are known for its excellent corrosion resistance of biocompatibility. Titanium metal forms a passive layer of TiO_2 on exposure to air & has superior corrosion resistance. Pure titanium and titanium alloys are widely used in making dental implants. In mouth, the crown placed over implant is usually made up of gold alloy (or) base metals like nickel-chromium alloy. The contact of dissimilar metals can create an electrolytic cell and may cause galvanic corrosion. To find out the corrosion behavior of pure titanium and titanium alloy when coupled with gold alloy and nickel-chromium alloy in artificial saliva with two different concentrations of Sodium Chloride. Corrosion behavior of Pure Titanium & Titanium Alloy coupled with Gold Alloy & Nickel Chromium alloy were studied by corrosion test, surface analysis and elemental release analysis in two different concentration solutions of sodium chloride (400 PPM & 1000 PPM). Nickel-chromium alloy specimens coupled with pure titanium and titanium alloy specimens showed severe pitting corrosion in artificial saliva containing both concentrations of sodium chloride. The data was analysed using IBM SPSS version 21 (SPSS version 21.0; IBM corporation, Armonk, NY, USA) statistical software. Pure titanium and titanium alloy specimens coupled with nickel chromium alloy specimens showed more corrosion in saliva with both concentrations of sodium chloride compared to gold alloy specimens indicating the use of gold alloy crowns for superstructure with pure titanium and titanium alloy implants.

Nano-Enabled Mitoxantrone Delivery Using Zirconium-Based Metal–Organic Frameworks: Evaluation in 3D Triple-Negative Breast Cancer Spheroids and Angiogenesis

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Abstract

Metal–organic frameworks (MOFs) are emerging nanomaterials for drug delivery owing to their tunable porosity, high surface area and potential for controlled drug release. Triple-negative breast cancer (TNBC) is an aggressive breast cancer subtype in which tumour architecture and angiogenesis contribute to therapeutic resistance. This study investigated the biological activity of mitoxantrone (MTX)-loaded zirconium-based MOF nanocarriers, UiO-66 and amino-functionalized UiO-66-NH₂, using physiologically relevant three-dimensional tumour and angiogenesis models. MTX-loaded UiO-66 and UiO-66-NH₂ nanocarriers, previously characterized for their physicochemical properties and drug-loading characteristics, were evaluated using 3D spheroids generated from TNBC cell lines MDA-MB-231 and MDA-MB-468, together with MCF-7 as a breast cancer comparison model. The effects of free MTX and MOF-based formulations on spheroid viability following treatment were assessed and compared with responses observed in 2D monolayer cultures. Anti-angiogenic activity was further investigated using a HUVEC–human fibroblast co-culture model. Tubule formation and junction numbers were quantified using fluorescence microscopy and image analysis. The 3D spheroid models demonstrated reduced sensitivity to MTX and its MOF-based formulations compared with corresponding monolayer cultures, highlighting the influence of tumour architecture on drug response. MTX-loaded UiO-66 retained cytotoxic activity in the 3D models, whereas the amino-functionalized formulation showed a comparatively reduced response in the spheroid system. In the angiogenesis model, free MTX inhibited endothelial tubule formation and network complexity. Both MTX-loaded MOF formulations retained anti-angiogenic activity, with responses broadly comparable to free MTX. The findings demonstrate the potential of zirconium-based MOF nanomaterials as carriers for MTX and highlight the importance of evaluating nanoformulations in advanced biological models. The integration of 3D TNBC spheroids with an endothelial–fibroblast angiogenesis model provides a more comprehensive approach for assessing the biological performance of MOF-based nanomedicines and their potential application in cancer therapy.

Keywords: Metal–organic frameworks; nanomaterials; UiO-66; UiO-66-NH₂; mitoxantrone; nano-drug delivery; triple-negative breast cancer; 3D tumour spheroids; angiogenesis.

A Prospective study on Drug related problems in Osteoarthritis Patients along with its comorbidities in a Tertiary Care Hospital. – An Observational Study

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Abstract

Osteoarthritis (OA) is a chronic, progressive joint disorder commonly affecting older adults and is frequently associated with comorbidities requiring multiple medications, increasing the risk of drug-related problems (DRPs). This study aimed to identify and classify DRPs among OA patients with comorbid condition. This is a six-month prospective observational study was conducted in the Orthopaedics Department of a tertiary care teaching hospital in Salem, Tamil Nadu. Fifty-two OA patients aged 18–69 years were included. Data were collected using a structured case report form. OA severity and pain were assessed using the Kellgren–Lawrence grading system and Visual Analogue Scale (VAS), respectively. DRPs were identified using the Pharmaceutical Care Network Europe (PCNE) classification system. Medication adherence and adverse drug reactions were also assessed. Most patients were aged 50–59 years (38%) and female (61%). Grade III/IV OA was observed in 78%, obesity in 52%, and severe pain in 58%. Hypertension (42%) and diabetes (29%) were common comorbidities. DRPs were identified in 30 (58%) patients, with treatment effectiveness problems (P1) predominating (83%). Drug selection (C1) was the major cause (67%). All patients showed high medication adherence, with no adverse drug reactions reported. OA grade was significantly associated with age, BMI and physical activity and strongly correlated with VAS ($\rho=0.896$, $p<0.001$). Systematic medication review and clinical pharmacist involvement may help optimize pharmacotherapy and reduce DRPs in OA patients.

Hydroxyapatite–Acacia Gum Nanocomposite with Antibacterial and Anti-Inflammatory Properties for Osteoarthritis Management and Bone Repair

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Abstract

Osteoarthritis is a common chronic joint disorder characterized by progressive deterioration of joint tissues, pain, swelling, reduced mobility and difficulty in performing daily activities. In advanced cases, when conventional drug treatment is not effective, total joint replacement may be required. Therefore, the development of improved biomaterials and therapeutic systems is important for orthopaedic applications. Hydroxyapatite (HAP) is a calcium phosphate ceramic that closely resembles the mineral component of natural bone. It is widely used in bone implants, surface coatings, and drug delivery systems. However, its limited antibacterial activity can restrict its applications. In this study, Acacia gum, a naturally derived polysaccharide, was incorporated into HAP to develop a HAP–Acacia gum nanocomposite using a wet-chemical synthesis method. The synthesized nanocomposite was characterized using FTIR, XRD, SEM, EDAX and TEM to determine its chemical structure, crystalline properties, surface morphology and elemental composition. Antibacterial activity was evaluated against Gram-negative *Escherichia coli* and Gram-positive *Staphylococcus aureus*. At 100 μ L of a 1 mg/mL suspension, inhibition zones of 16 mm and 17 mm were observed, respectively. The anti-inflammatory activity was evaluated in LPS-stimulated RAW 264.7 macrophages using the MTT assay. The nanocomposite showed dose-dependent inhibition of LPS-induced inflammation, with inhibition values of 22%, 41%, 60%, 87%, 96%, and 100% at 10, 20, 30, 40, 50, and 60 μ g/mL, respectively. The IC₅₀ was found to be 24.22 μ g/mL. Together, these findings indicate that HAP–Acacia gum nanocomposites combine antibacterial and anti-inflammatory properties and may support future approaches to osteoarthritis management and bone repair.

Keywords: Osteoarthritis, Hydroxyapatite-Acacia gum, Nanocomposite, Antibacterial, Anti-inflammatory

Microwave-Assisted Green Synthesis of Bacterial Carbon Nanodots and Evaluation of Their Biological Properties for Various Applications

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Abstract

Carbon nanodots (CNDs) have emerged as multipurposed fluorescent nanomaterials with low acute toxicity having broad biomedical potential. This study reports a rapid, eco-friendly, microwave-assisted green synthesis of CNDs using bacterial cell-free supernatant supplemented with citric acid and D-glucose as co-carbon precursors. Successful microwave assisted synthesis was confirmed by a characteristic colour change from pale yellow to light brown and fluorescence emission under UV irradiation (365 nm). UV-Visible spectroscopy revealed a characteristic π - π^* absorption peak at 270.4 nm (absorbance value of 3.088), consistent with sp²-hybridized graphitic carbon core formation. FTIR spectroscopy identified 21 distinct peaks, with key absorptions confirming carboxylate (1431.25 cm⁻¹), carbonyl (1733.85 cm⁻¹), aromatic C=C (1617.69 cm⁻¹), and amide II N-H (1537.38 cm⁻¹) surface functionalities, providing evidence for N-doped surface chemistry. This core-shell configuration is the universal chemical signature of N-doped carbon nanodots. Comparative antimicrobial evaluation of Green synthesized CNDs with Chemically synthesized CNDs by agar well diffusion method against five clinically relevant pathogens — *Staphylococcus* spp., *Streptococcus* spp., *Escherichia* spp., *Klebsiella* spp., and *Pseudomonas* spp. — demonstrated moderate broad-spectrum activity in the former, the latter being higher. Minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) were determined by microdilution method using MIC broth for the pathogens. All the tested pathogens showed minimum inhibitory concentration at 200 μ l/mL where upon they exhibited bactericidal activity for only *E.coli* and *Pseudomonas* spp., alone. Antibiofilm activity assessed by Crystal violet assay showed CND based concentration-dependent inhibition, with all tested pathogens exhibiting inhibition of 100% at 200 μ g/mL. Antioxidant potential evaluated by DPPH assay demonstrated dose-dependent free radical scavenging activity (8.31%–17.60% at 100–500 μ g/mL). A chitosan–CND composite coating applied by dip-coating method, effectively reduced surface microbial colonization on glass slides up to the tested two weeks. These findings establish bacterial supernatant as a novel biogenic precursor for multifunctional N-doped CNDs with promising antimicrobial and antibiofilm activities which can be useful in surface-coating applications in medical and industrial and various other fields. The bacterial supernatant, rich in extracellular proteins, amino acids, and polysaccharides should have served as both the primary carbon source and a natural nitrogen-doping agent, producing nitrogen-doped CNDs. This study proposes a synthesis of biologically useful CNDs without any toxic reagents or specialized equipment in an ecofriendly method.

Keywords: N-doped Carbon nanodots, Microwave-assisted green synthesis, Antimicrobial and antibiofilm activity, Chitosan–CND composite coating, DPPH antioxidant activity.

Digital-Exposure Gradients in OSDI-Defined Symptomatic Dry Eye Among Medical Trainees: A Translational Pathway Toward Tear-Film Spectroscopy

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Abstract

Digital visual load is increasingly relevant to ocular-surface health, but symptom burden across medical training stages remains incompletely characterized. We assessed OSDI-defined symptomatic dry eye, digital-exposure gradients, functional burden, and care seeking among medical trainees. This cross-sectional study included 200 adults (100 MBBS students and 100 postgraduate residents). Participants completed the OSDI-12 and a structured questionnaire on screen duration, uninterrupted use, break behaviour, sleep, stress, and ocular allergy/rubbing. OSDI >12 defined symptomatic dry eye. Modified Poisson regression estimated adjusted prevalence ratios. Symptomatic dry eye affected 112/200 participants (56.0%; 95% CI 49.1-62.7%), with identical prevalence in both training groups. Prevalence increased from 18.8% at 2-<4 h/day to 82.6% at ≥ 8 h/day of screen exposure, from 15.0% with <30 min to 84.6% with >2 h uninterrupted use, and from 26.8% with 20-30-min breaks to 81.0% with rare breaks (all $p < 0.001$). Severe OSDI scores occurred in 29.5%; 96.6% of this subgroup reported moderate/severe work-study interference, yet only 25.4% had consulted an ophthalmologist. Greater screen exposure, uninterrupted use, delayed breaks, shorter sleep, higher stress, and ocular allergy/rubbing remained independently associated. Medical trainees showed substantial, behaviour-linked dry-eye symptom burden and a marked care-seeking gap. These findings provide an exposure-stratified foundation for an IEC-approved translational extension integrating TBUT, Schirmer testing, tear UV-Visible spectroscopy, HbA1c, and OCT macular thickness to investigate non-invasive tear spectral signatures across anterior and posterior diabetic ocular changes.

Keywords: Dry eye; OSDI; digital screen exposure; tear film; UV-Visible spectroscopy; optical coherence tomography.

Hydrolyzed Eggshell Membrane–Calcium Chelation Complex for Enhanced Antimicrobial Activity, Antioxidant Defense and Male Reproductive Homeostasis Function

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Abstract

Male infertility is strongly associated with oxidative stress–induced damage to sperm structure and function, necessitating bioactive systems capable of regulating redox balance and calcium homeostasis. In this study, a peptide–Ca²⁺ chelated eggshell membrane system (Eh-ESM–Ca) was developed via enzymatic hydrolysis and compared with adsorption-based unhydrolyzed ESM–Ca (u-ESM–Ca). To the best of our knowledge, this is the first report of a hydrolyzed ESM–Ca chelation complex (Eh-ESM–Ca) for reproductive biomedical applications. Spectroscopic analyses (UV–Vis, FTIR, XPS) confirmed strong coordination between Ca²⁺ ions and peptide functional groups (–COO[–], –NH₂), while morphological studies revealed a transition from fibrous u-ESM to a homogeneous peptide–Ca network with improved solubility and bioavailability. Biologically, Eh-ESM–Ca demonstrated superior antioxidant activity, significantly reducing reactive oxygen species (ROS). In vitro sperm studies showed improved viability (~84%), morphology (~87%), and motility, along with reduced DNA damage under oxidative stress compared to u-ESM–Ca. In vivo results further confirmed excellent systemic safety, with normal liver (AST, ALT) and kidney (urea, creatinine) markers, enhanced catalase activity, and reduced lipid peroxidation. Reproductive parameters, including testosterone levels and spermatogenesis, were significantly improved. The enhanced performance is attributed to the synergistic interaction of bioactive peptides, metabolites, and Ca²⁺, enabling calcium-containing peptide complex and redox regulation. This study presents a multifunctional, biocompatible platform for advanced reproductive and biomedical applications.

Keywords: Eggshell membrane; Calcium bioavailability; Redox homeostasis; Antioxidant peptides; Male infertility

Development And Characterization of Banana Stem Fibre Reinforced PVA-Based Calorimetric Hydrogel with Red Cabbage Extract for Diabetic Wound Healing

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Abstract

Diabetic wounds are chronic conditions characterised by delayed tissue regeneration and healing, increased oxidative stress, and susceptibility to infections. Traditional wound dressings often provide limited therapeutic benefits, creating a need for multifunctional biomaterials that support the wound microenvironment for healing. This study aims to develop a polyvinyl alcohol (PVA)-based colorimetric hydrogel scaffold reinforced with banana stem fibre for potential application in diabetic wound management. Natural red cabbage extract rich in anthocyanins acts as a pH indicator of the colorimetric hydrogel. The physiological milieu of the infected wound will be alkaline compared to the healthy skin, which is indicated by the colour change of the gel while changing the dressing. Different concentrations of PVA and glutaraldehyde were evaluated to determine the optimal formulation. The resulting hydrogels were evaluated for gelation, homogeneity, structural integrity, flexibility, and swelling ability. The results demonstrated that increasing the PVA concentration improved gel formation and stability. Among the tested formulations, the hydrogel containing 3% PVA and 1 mL glutaraldehyde exhibited the most favourable properties, including good mechanical integrity, uniformity, flexibility, and swelling ability. Furthermore, incorporation of banana stem fibre introduced into the gel provides the mechanical strength of wound dressing in addition to its regenerative property. Overall, the developed PVA-based hydrogel scaffold demonstrates promising potential as a multifunctional wound dressing for diabetic wound management.

Keywords: Diabetic wounds; PVA hydrogel; Banana stem fibre; Red cabbage extract; pH Responsive Antioxidant activity; Tissue Regeneration; Wound dressing; Biomaterial scaffold.

Designing and Fabrication of Multifunctional Bi (III) Complexes for Biomedical, Catalytic and Functional Applications

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Abstract

The present study focuses on the design, synthesis and characterization of novel bismuth (III) metal complexes containing multifunctional organic ligands and explores their potential applications in biomedical and functional materials chemistry. Bismuth is an attractive metal centre because of its distinctive coordination chemistry, accessible oxidation state, relatively low toxicity and promising biological properties. A series of Bi (III) complexes will be synthesized using carefully selected N, O-, N, S- and O, S-donor ligands to investigate the influence of ligand architecture on their structural and functional properties. The synthesized complexes will be characterized using elemental analysis, FT-IR, UV–Visible spectroscopy, NMR spectroscopy, mass spectrometry, thermal analysis, powder X-ray diffraction and single-crystal X-ray diffraction, wherever feasible. Their biological potential will be evaluated through antibacterial, antifungal, antioxidant and cytotoxicity studies. In addition, molecular docking and computational studies will be employed to understand possible metal–ligand interactions and structure–activity relationships. The complexes may also be explored for catalytic, sensing and photocatalytic applications, demonstrating the multifunctional nature of bismuth coordination compounds. The proposed investigation is expected to establish useful correlations between molecular structure, coordination environment and biological/functional activity, thereby contributing to the development of new bismuth-based materials with potential applications in medicinal chemistry, catalysis, sensing and environmental remediation.

Keywords: Bismuth (III) complexes; Multifunctional ligands; Antimicrobial activity; Antioxidant activity; Cytotoxicity; Molecular docking

Wireless Optogenetically-Activated Living Hydrogels: Agro-Industrial Waste-Derived Carbon Quantum Dots for Light-Driven Neural Regeneration

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Abstract

Regeneration of critical-sized neural defects resulting from traumatic spinal cord injuries or peripheral nerve transections remains a profound challenge in regenerative medicine due to the intrinsic inability of mature mammalian nerves to bridge macro-gaps without external biophysical guidance. Conventional nerve guidance conduits offer passive structural support but lack the dynamic electrical and biochemical cues required to actively drive axon elongation and overcome fibrotic inhibitory barriers. Here, we present a wireless, light-driven therapeutic paradigm utilizing optogenetically activated living hydrogels powered by green-synthesized carbon quantum dots (CQDs) for accelerated neural regeneration. We developed an injectable, biomimetic silk fibroin hydrogel matrix embedded with highly biocompatible CQDs synthesized via a green, bottom-up thermal process from abundant agro-industrial plant waste. Under transdermal illumination, these green-derived CQDs act as wireless intra-tissue nano-transceivers, absorbing deep-tissue-penetrating near-infrared (NIR) light and converting it into localized visible photoluminescence and micro-volt electrical fields. This non-invasive biophysical stimulation acts via photobiomodulation and local bioelectronic conversion to activate voltage-gated calcium channels and intrinsic repair pathways within migrating neural cells. Empirical and predictive modeling demonstrate that this electroactive matrix achieves an ideal conductivity window (~ 0.05 S/m), leading to a significant increase in Schwann cell migration and a three-fold acceleration in functional axon alignment across critical nerve gaps. Furthermore, the degradation kinetics of the silk matrix are synchronized with native tissue remodeling, resolving into non-toxic metabolites as functional neural circuits are restored. By upcycling agricultural waste into sophisticated wireless bioelectronics, this platform establishes a sustainable, highly personalized strategy for non-invasive neural repair.

Keywords: Green Nanotechnology; Carbon Quantum Dots; Neural Regeneration; Wireless Optogenetics; Agro-Industrial Waste; Silk Fibroin Hydrogels.

Synthesis and Physicochemical Characterization of Hydroxyapatite–Rutin Nanocomposite for Antibacterial Applications: An Experimental and Molecular Docking Study

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Abstract

Hydroxyapatite (HAP) is an important calcium phosphate biomaterial owing to its biocompatibility, bioactivity and biomimetic to the mineral component of bone. The incorporation of bioactive molecules into HAP provides an approach for developing multifunctional nanomaterials with additional biological properties. In the present study rutin functionalized hydroxyapatite (HAP–rutin) nanocomposite was synthesized using an ultrasonic-assisted wet-chemical precipitation method. Rutin was incorporated at four different concentrations (0.1, 0.3, 0.5 0.7 wt.%) during the synthesis of HAP to obtain a nanocomposite with enhanced functional characteristics and antibacterial potential. The use of ultrasonic assistance facilitated effective mixing of the reaction components during precipitation and supported the formation of the HAP–rutin nanocomposite. The synthesized HAP–rutin nanocomposite was characterized by Fourier Transform Infrared (FTIR) Spectroscopy, X-ray diffraction (XRD) and Field-Emission Scanning Electron Microscopy (FESEM). FTIR analysis confirmed the characteristic functional groups of hydroxyapatite and the presence of rutin-associated functional groups indicating the incorporation of rutin into the HAP matrix. XRD analysis confirmed the formation of the HAP crystalline phase and provided information on the structural characteristics of the synthesized nanocomposite. FESEM analysis revealed a predominantly spherical morphology with a porous structure in the HAP–rutin nanocomposite. In addition the antibacterial activity of the synthesized HAP–rutin nanocomposite was assessed against the Gram-positive bacterium *Staphylococcus aureus* and the Gram-negative bacterium *Escherichia coli*. The observed antibacterial activity of the HAP–rutin nanocomposite highlights the contribution of rutin incorporation to the biological functionality of the HAP matrix. Molecular docking studies were performed to investigate the binding interaction of rutin with selected bacterial targets namely *Staphylococcus aureus* (PDB ID: 4NPF) and *Escherichia coli* (PDB ID: 4KFG). Rutin exhibited binding energies of –11.52 and –7.22 kcal/mol against *S. aureus* and *E. coli* targets respectively indicating favorable molecular interactions with both bacterial proteins. The present findings demonstrate that ultrasonic-assisted wet-chemical precipitation can be employed to synthesize HAP–rutin nanocomposite with defined structural and morphological characteristics, antibacterial activity and favorable molecular interactions. The synthesized HAP–rutin nanocomposite represents a promising material for further investigation in various biomedical applications.

Keywords: Hydroxyapatite; Rutin; Nanocomposite; Molecular docking; Antibacterial activity

Silver Nanoparticle and Peptide Drug-Loaded Smart Nanocomposite Hydrogel Scaffold for Enhanced Diabetic Wound Healing

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Abstract

Diabetic wounds are characterized by delayed healing, persistent inflammation, and increased susceptibility to bacterial infections. Developing multifunctional biomaterials that provide sustained antimicrobial activity may improve wound healing. This study aimed to develop and evaluate a smart composite hydrogel scaffold incorporating a peptide drug and silver nanoparticles (Ag-NPs) for diabetic wound management. We prepared the gramicidin-loaded Ag-NP hydrogel scaffold using biocompatible polymers and evaluated its physicochemical and structural characteristics. The wound-healing performance and biocompatibility of the optimized scaffold were further assessed in a diabetic wound model. The developed hydrogel exhibited a porous and interconnected structure with favorable swelling, moisture retention, and mechanical properties. FTIR and XRD analyses indicated compatibility and successful incorporation of gramicidin and Ag-NPs within the hydrogel matrix. The scaffold provided sustained release of gramicidin and demonstrated enhanced antibacterial activity against both *S. aureus* and *P. aeruginosa*. In the diabetic wound model, the optimized scaffold showed favorable biocompatibility and improved wound-healing characteristics.

Keywords: Nanoparticle; Antimicrobial peptide; Composite hydrogel patches; Wound Healing.

Bacterial-Assisted CuO Nps for Effective Removal of MDR Strains and Synthetically Prepared Ciprofloxacin

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Abstract

The Global rise of antibiotic contamination in pharmaceutical waste water and multidrug-resistant (MDR) pathogens demands remediation strategies that address both problems simultaneously. The objective of this study aims for removal efficiency of MDR pathogens and Ciprofloxacin from synthetic aqueous solution by using Bacterial synthesizing CuO NPs. Out of 20 bacterial isolates, eight were primarily identified as Cu(II)-tolerant strains, of which MR17 and MR14 showed the highest potential in synthesizing CuO NPs, as physical evidenced by the formation of stable green precipitates. The Biosynthesized CuO NPs were characterized by UV-Visible Spectroscopy, FTIR, XRD and SEM-EDX. The MR14 and MR17 derived CuO NPs were evaluated for their capability to remove the antibiotic Ciprofloxacin from aqueous solution which results that MR14 CuO NPs removed 80% within 30mins than MR17 CuO NPs removed only about 20%. In addition, the antibacterial activity of the synthesized CuO NPs were tested against six clinically relevant MDR strains. MR14 derived CuO NPs exhibited larger zone of inhibition than MR17 CuO NPs by agar well diffusion assay. The Nanoparticle synthesized from MR14 was selected as a potential CuO NPs that removes Ciprofloxacin and has strong antibacterial activity against MDR strains. It also exhibited up to 80% DPPH radical scavenging at 100 µg/mL. The batch studies were conducted to assess the removal of Ciprofloxacin to determine the optimum parameters, CuO NPs removed up to 98% of ciprofloxacin within 120 minutes, with optimal performance at higher nanoparticle loading (100µg), neutral pH and 40–45 °C. Finally, the application studies were done by incorporation of CuO NPs into Cellulose acetate (CA+CuO) membrane achieved 89% removal of MDR strains and 98% removal of Ciprofloxacin. This study reveals that (CA+CuO) membrane as a promising solution for addressing water contamination challenges in environmental and public health concerns

Key Words: CuO NPs, Ciprofloxacin, MDR strains, Bacterial synthesis, Cellulose acetate, CA+CuO membrane.

Chitosan Nanoparticle-Based Nano formulation of 1,2,4-Triazole–Piperazine Hybrids for Enhanced Anticancer Activity: An Integrated Experimental and Computational Study

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Abstract

The development of nanotechnology-enabled drug delivery systems offers a promising strategy for improving the biological performance of anticancer agents. In this study, a series of 1,2,4-triazole–piperazine hybrid cinnamamide derivatives (M1-M11) were synthesized and characterized using FT-IR, ¹H/¹³C NMR, HRMS and single-crystal X-ray diffraction. The synthesized compounds were evaluated for antioxidant activity by the DPPH assay and for in vitro cytotoxicity against MCF-7 breast cancer cells, with HEK-293T cells used as a normal-cell reference. Among the synthesized derivatives, M2 showed the highest anticancer activity in the free-compound series, with an IC₅₀ of 98.67 μM. Molecular docking against the breast cancer-associated target protein 3ERT showed favourable binding affinities, while molecular dynamics simulation supported the stability of the M2–3ERT complex. To improve the delivery performance of the active compounds, M2, M3 and M4 were incorporated into chitosan nanoparticles through ionic gelation using sodium tripolyphosphate as a crosslinking agent. The resulting nanoformulations showed nanoscale particle sizes of 34-52 nm and high encapsulation efficiencies of approximately 89%. DLS, FT-IR, XRD, SEM and TEM analyses were used to characterize the nanoformulations. Importantly, nanoencapsulation substantially enhanced the cytotoxic activity against MCF-7 cells, with M4-CSNP showing an IC₅₀ of 7.89 μg/mL. Chitosan-based nanoformulation therefore provides a nanotechnology-oriented approach for improving the anticancer performance of heterocyclic compounds. The study integrates medicinal chemistry, nanotechnology, biological evaluation and computational modelling, highlighting its relevance to biomedical and healthcare applications.

Etiology Study on Dry Eye Syndrome and Its Management in A Tertiary Care Hospital- An Observational Study

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Abstract

Dry Eye Disease (DED) is a multifactorial ocular surface disorder characterized by tear-film instability, ocular discomfort, and visual disturbances. It may be associated with systemic diseases, medications, environmental exposure, ageing, prolonged screen time, and ocular factors. A prospective observational study was conducted in a period of 6 months in the Department of Ophthalmology. 120 patients above the age of 18 years with symptoms suggestive of Dry Eye Disease were recruited into the study. The data pertaining to the patient's demographics, ocular symptoms, associated systemic diseases, medications and the environmental exposure, screen time and ocular history were recorded. The patients were classified based on their tear film status into aqueous deficient, evaporative and mixed type of dry eye. The severity of dry eye was analyzed using the Ocular Surface Disease Index questionnaire and the management was recorded along with the improvement in the associated symptoms. Out of 120 patients, 62(52%) were males while 58(48%) were females. The most common type of symptoms was recurrent symptoms which were reported by 70(58%) patients. 42(35%) patients each had aqueous-deficient and mixed dry eye while 36(30%) had evaporative dry eye. The most common presentations were eye fatigue 65%, redness 64%, blurred vision 59%, and foreign-body sensation 58%. Using the OSDI score, 73(61%) patients had moderate Dry Eye Disease, 32(27%) had severe while 15(13%) had mild Dry Eye Disease. This study showed that Dry Eye Disease occurs due to a range of systemic, ocular, environmental, lifestyle and medication factors. The assessment of severity using OSDI score showed that moderate severity was more prevalent compared to other levels of severity among the study participants. The identification of associated factors and the early assessment of severity, proper management, lifestyle changes and patient counselling will improve patient comfort.

Keywords: Dry Eye Syndrome, Etiological Factors, OSDI, Dry Eye Severity, Risk Factors, Management, Ophthalmology, Lubricant Eye Drops.

OP-BM-98

Synthesis, Characterization and Dual Catalytic-Antibacterial Applications of Reduced Graphene Oxide-Supported Cobalt-Nickel Nanocomposites

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Abstract

The precise control over nanoparticle size, morphology, and matrix support is essential for tailoring their physical, chemical, and biological performance. Here, we report the synthesis and characterization of graphene oxide-supported cobalt (Co), nickel (Ni), and bimetallic cobalt-nickel (Co-Ni/rGO) nanoparticles. The functional group integration, phase purity, crystalline structure, and optical properties were thoroughly investigated using Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), and UV-Visible Spectroscopy. Furthermore, the catalytic efficacy toward organic pollutant reduction and the antibacterial activity against targeted bacterial strains were evaluated. The Co-Ni/rGO nanocomposite displayed enhanced performance in both environmental pollutant degradation and antimicrobial inhibition compared to monometallic formulations, demonstrating its promise as a versatile, biologically active nanomaterial for multi-functional applications.

Keywords: Cobalt-Nickel Nanoparticles, Graphene Oxide, Methylene Blue, Catalysis, Antibacterial Activity, Environmental Remediation

Preparation of Nano-Metal Complex of Benzilic acid and Its Antibacterial Activity

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technology and Advanced studies*

Abstract

Benzilic acid and its derivatives possess versatile coordination properties and have attracted considerable interest because of their potential biological applications. In the present study, a nano-metal complex of benzilic acid was prepared by the reaction of benzilic acid with a suitable transition-metal salt under controlled conditions. The synthesized complex was characterized using spectroscopic and physicochemical techniques, including UV–Visible spectroscopy, FTIR, $^1\text{H}/^{13}\text{C}$ NMR spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM), to confirm its molecular structure, crystalline nature, and nanoscale morphology. The formation of the metal complex resulted in significant changes in the characteristic spectral features of benzilic acid, indicating coordination of the ligand with the metal ion. The antibacterial activity of the synthesized nano-metal complex was evaluated against selected Gram-positive and Gram-negative bacterial strains using the agar disc diffusion and minimum inhibitory concentration (MIC) methods. The nano-metal complex exhibited enhanced antibacterial activity compared with the free benzilic acid ligand, which may be attributed to the combined effect of metal-ion coordination and nanoscale particle size, providing increased surface interaction with bacterial cells. The results demonstrate that nano-metal complexes of benzilic acid have promising antibacterial properties and may serve as potential candidates for the development of novel antimicrobial materials.

Keywords: Benzilic acid; Nano-metal complex; Metal coordination; Nanoparticles; Characterization; Antibacterial activity; MIC.

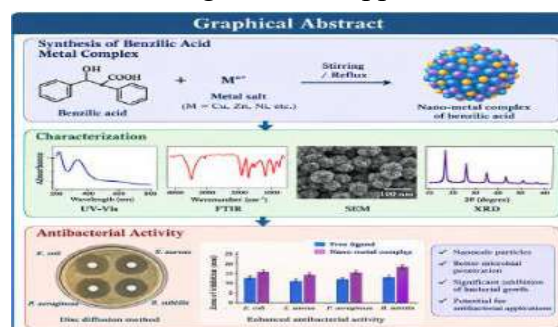
Marine Biowaste-Derived Sr/Zr Co-Doped Hydroxyapatite with Improved Bioactivity for Bone Tissue Regeneration

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Abstract

The development of sustainable and bioactive materials from marine biowaste offers a promising approach for bone regeneration while addressing the environmental challenges associated with waste disposal. In this study, hydroxyapatite (HAp) was derived from clam shell marine biowaste and co-doped with strontium (Sr) and zirconium (Zr) to enhance its physicochemical and biological properties for potential bone regeneration applications. The incorporation of Sr and Zr was designed to improve the bioactivity, structural stability, and biological functionality of the biowaste-derived HAp. The synthesized Sr/Zr co-doped HAp was systematically characterized to investigate its phase composition, crystallinity, morphology, elemental distribution and surface characteristics. The formation of the HAp phase and successful incorporation of the dopant elements were evaluated using complementary physicochemical characterization techniques. The bioactivity of the synthesized material was assessed based on its apatite-forming ability and interaction with biological environments. Sr incorporation is expected to promote osteogenic activity and bone mineral formation, while Zr contributes to structural stability and improved material performance. The combined effects of Sr and Zr provide a multifunctional HAp-based biomaterial with enhanced characteristics compared with undoped HAp. Overall, this study demonstrates the potential of marine biowaste-derived Sr/Zr co-doped HAp as a sustainable and bioactive biomaterial for bone regeneration and related orthopedic applications, while simultaneously providing a value-added pathway for the utilization of marine shell waste.



Key words: Marine biowaste, Clam shell-derived biomaterial, Bioactive ceramics, Osteogenesis, Orthopedic implants.

Assessing Inhaler Technique Errors and the Impact of Pharmacist-Led Education on Patient Outcomes of COPD and Asthma

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Abstract

Asthma and chronic obstructive pulmonary disease (COPD) are chronic respiratory diseases in which inhaled medicines are central to treatment. Their effectiveness depends on correct device handling and medication adherence. Incorrect metered-dose inhaler (MDI) and dry powder inhaler (DPI) technique may reduce drug delivery and contribute to poor symptom control and exacerbations. To assess inhaler technique errors among patients with asthma and COPD and evaluate the effect of pharmacist-led education on inhaler technique and patient outcomes. A prospective interventional study was conducted over 6 months at a tertiary care hospital in Salem among 92 adults with asthma or COPD prescribed DPI or MDI therapy. Participants underwent structured assessment of inhaler technique, medication adherence using the Morisky scale, disease-control measures, and exacerbation history. DPI technique was assessed using 7 steps and MDI technique using 8 steps. The pharmacist identified errors, explained the correct sequence, demonstrated device use, obtained return-demonstration, and reinforced correct technique. Pre- and post-intervention changes were evaluated using paired statistical tests; categorical associations were assessed using chi-square testing, with $p < 0.05$ considered significant. Among 92 participants, 44 used DPI and 48 used MDI. Inhaler technique improved significantly in both DPI and MDI users ($p < 0.001$ for each). Medication adherence also improved significantly in both groups ($p < 0.001$). Occupation was significantly associated with exacerbation frequency ($p = 0.006$), whereas educational level was not significantly associated with pre/post assessment scores ($p = 0.552$). Pharmacist-led education improved inhaler technique and medication adherence in asthma and COPD patients. Routine assessment, demonstration, return-demonstration, and periodic reinforcement may support effective inhaler use and respiratory self-management.

Key words: Asthma, Chronic Obstructive Pulmonary Disease, Inhaler technique, Dry powder Inhaler, Metered-dose Inhaler, Pharmacist-Led Education, Patient Counselling, Medication Adherence, Respiratory Outcomes, Inhaler Technique Errors.

Computational Studies on the Structural Preferences of Psilocybin Derivatives

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Abstract

Psilocybin mushrooms usually known as Magic Mushrooms, present in varying concentration in about 200 species. They are commonly known for their hallucinating property and used as recreational drugs. One of the important chemical compounds present in magic mushrooms is psilocybin which is a classical hallucinogen. Psilocybin is a tryptamine natural product found in magic mushrooms. It is zwitter ionic in nature and converted to psilocin when entered into the body. Psilocin is responsible for the psychoactive nature of these mushrooms. Though the psychoactive effect of these magic mushrooms has been known from biological studies, the exact mechanism at molecular level in brain is not known so far. Here, we have attempted to study the mechanism of this Psychoactivity of psilocybin at molecular level. Initially, we have computed the electronic and geometrical structure as well as spectroscopic properties of the important chemical compound's psilocybin, psilocin and their derivatives. Computational chemistry tools like DFT (BP86/TZVP) calculations are proved to be successful in studying and modelling chemical compounds. DFT (BP86/TZVP) optimized geometries are found to be minima in potential energy surface and in close agreement with the experimental values for the known compounds. Molecular orbital analysis is helpful in predicting and understanding the nature of these compounds. DFT computations to study the mechanism of the formation of these psychoactive molecules are in progress. The important preliminary results obtained will be presented. Also, psilocybin provides major benefits for cancer patients, ranging from preventing severe chemotherapy side effects to treating emotional distress.

Keywords: Psilocybin, Psilocin, DFT, Psychoactivity, Molecular orbitals

**Additive Manufacturing of Centrifugal Pump Impellers Based on
Nanocomposite Polymer Materials: Hydraulic Performance and
Sustainable Manufacturing Aspects**

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Abstract

Centrifugal pumps have been extensively used in water supply systems, irrigation, industrial processes, and power plants. The role of impeller in the process of conversion of hydraulic energy is essential. The fabrication of conventional metallic impellers requires relatively complicated manufacturing processes, significant material consumption and constraints in quick changes in the design. Additive manufacturing represents an alternative approach for the production of complex geometrical impellers with the reduction of material waste, development cycle time and high design freedom. This paper provides a critical review on the use of polymer and nanocomposite materials in the fabrication of the centrifugal pump impellers through additive manufacturing, focusing on the material properties, the manufacturing parameters, the mechanical performance, surface quality and hydraulic performance of the fabricated impellers. Special attention is paid to nanocomposites and reinforced polymers due to the possibility of improvement in stiffness, strength, wear resistance and dimensional stability compared to the non-reinforced polymers. The effect of the material composition, reinforcement, layer orientation, infill density, printing parameters and surface quality on the performance of the impellers is considered. The correlation between material properties and hydraulic parameters, including head, discharge, torque, power consumption and efficiency, is analyzed. This review highlights research gaps and suggests a framework for developing nanocomposites and testing them for hydraulic performance within sustainable centrifugal pumps.

Keywords: Centrifugal Pump, Impeller, Nanocomposites, Additive Manufacturing, Polymer Composites, Hydraulic Performance.

Passive Acoustic Implants for Biofilm & Micro-Fracture Detection

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Abstract

Colonization of the implant surface by bacteria and the occurrence of micro-fractures in the implant or bone–implant interface are two critical failure mechanisms of orthopaedic and dental implants. These conditions can go undetected until they cause a serious infection, loosening, or mechanical failure. Conventional practices such as radiography, blood-marker analysis and clinical examination can only detect problems at a point where there has been significant tissue degradation, and repeated imaging or biological sampling is impractical for continuous monitoring. This work is a proposal of passive acoustic implant schemes for long-term, battery-free, in-situ monitoring of biofilm formation and micro-fracture initiation. The idea is to use a resonant acoustic structure, such as a surface acoustic wave or piezoelectric resonator, within or attached to the implant that can be interrogated via a wireless means with an external transducer or coil. As the accumulations of biofilm and structural changes occur, changes in the acoustic response should be distinguishable. An increase in the mass of the biofilm may lead to a greater damping, and changes to the resonance frequency, while micro-fractures can result in new resonance components and harmonic scattering. Thus, the potential for signal-processing approaches that enable the identification of changes in the surface characteristics as compared to structural damage in the reflected acoustic spectrum can be explored. The designs of resonators, biocompatible materials, wireless interrogation, acoustic signal processing, and long-term hermetic packaging will be investigated. Some of the major issues are tissue dependent read range, biocompatibility, false positive due to normal tissue remodeling and experimental validation in a controlled fracture model and in-vitro biofilm model. This method may allow for more timely and regular assessment of implant integrity and infection risk, leading to timely clinical interventions before significant implant failure.

Keywords: Acoustic Sensors; Biofilm Detection; Micro-Fracture Detection; Implantable Devices.

Bioactive Compounds from *Inula racemosa* for Biomedical Applications in Alzheimer's Disease

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Abstract

Alzheimer's disease (AD) remains a critical challenge in modern biomedical research, demanding novel therapeutic leads capable of modulating complex, multi-target neurodegenerative pathways. Natural products offer a rich reservoir of structurally diverse bioactive compounds to meet this need. This study evaluates the biomedical potential of *Inula racemosa* (Asteraceae), a medicinal plant traditionally valued for its therapeutic properties, by focusing on the isolation, structural characterization, and neuroprotective evaluation of its secondary metabolites. Root extracts will be prepared via sequential solvent extraction and subjected to bioactivity-guided fractionation using advanced chromatographic techniques. The isolated active constituents will be structurally characterized using FTIR, NMR, GC-MS, and LC-MS. To determine therapeutic efficacy against AD pathogenesis, the compounds will be screened via in-vitro assays measuring acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) inhibition, free radical scavenging activity, and neuroprotective capacity against induced cellular toxicity. Ultimately, these findings will elucidate the chemical profile of *I. racemosa* and provide key mechanistic insights into its bioactive constituents, establishing a baseline for targeted, natural small-molecule drug design strategies in neurodegenerative disease management.

Keywords: *Inula racemosa*, Alzheimer's disease, Neuroprotection, Bioactivity-guided fractionation, Acetylcholinesterase inhibition.

**Cerium - Selenium Co-Substituted Hydroxyapatite: Structural,
Morphological and Antibacterial properties for Biomedical
Applications**

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Abstract

Hydroxyapatite (HAp) is a bioactive ceramic material that resembles the mineral components of natural bone and teeth. It is a potential biomaterial which is widely used in biomedical application due to its biocompatibility and non-toxicity property. However, it has some limitations including poor mechanical strength and low antibacterial activity which can be improved by elemental substitution. In this work, cerium and selenium co-substituted hydroxyapatite (Ce-Se HAp) was synthesized by hydrothermal method, with the aim of improving its functional properties and antibacterial activity. The prepared powder was characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM–EDS). Based on XRD result the formation of HAp was confirmed by the characteristic diffraction peaks corresponding to the crystalline hydroxyapatite phase. FTIR analysis showed the characteristic functional group and SEM analysis revealed the morphology of the synthesized Ce-Se HAp with agglomerated flakes and rod-like structures. EDS result confirmed the presence of calcium, phosphate, cerium and selenium in the synthesized sample. The antibacterial activity was evaluated against clinically relevant bacteria *Escherichia coli*, and *Staphylococcus aureus* and the results showed that the synthesized material has the potential antibacterial properties towards both Gram-positive and Gram-negative bacterial strains.

Keywords: Substituted Hydroxyapatite; Hydrothermal synthesis; XRD; Antibacterial activity; Biomedical applications.

Heat-Assisted Synthesis, Structural Characterization and Biological Evaluation of a Silver(I) Schiff Base Complex

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Abstract

A novel Schiff base ligand was synthesized through the condensation reaction of aniline with glutaraldehyde and subsequently coordinated with silver(I) ions using silver nitrate to obtain a silver(I) Schiff base metal complex. The formation of the Schiff base ligand and its silver(I) complex was investigated using various physicochemical and spectroscopic techniques. Fourier-transform infrared (FTIR) spectroscopy was employed to identify the characteristic functional groups and confirm the coordination of the ligand with the silver ion. The structural features of the synthesized ligand and metal complex were further investigated using ¹H and ¹³C Nuclear magnetic resonance (NMR) spectroscopy. The surface morphology and Elemental composition were examined by scanning electron microscopy coupled with Energy-dispersive X-ray spectroscopy (SEM-EDX), while the crystalline nature and phase characteristics were evaluated using X-ray diffraction (XRD) analysis. Furthermore, the synthesized Schiff base ligand and silver(I) complex were evaluated for their antimicrobial and anticancer activities. The biological studies demonstrated the potential of the silver(I) Schiff base complex as a biologically active coordination compound. The enhanced biological activity of the silver(I) complex may be associated with the coordination of the Schiff base ligand to the silver ion, which can modify the physicochemical and biological properties of the ligand. Overall the synthesized silver(I) Schiff base complex presents a promising candidate for further investigation in antimicrobial and anticancer applications.

Keywords: Aniline; Glutaraldehyde; Silver nitrate, Anti-microbial activity, Anticancer activity.

Investigation of a Carboxymethyl Cellulose-Lignin-Vanillin Wound Dressing for Diabetic Wound Healing

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Abstract

Diabetic wounds remain a significant healthcare challenge due to impaired tissue regeneration and increased susceptibility to infection. The current study aimed to isolate cellulose (CEL) and lignin (LIG) from sugarcane bagasse, prepare carboxymethyl cellulose (CMC) from CEL, and incorporate the bioactive compound vanillin (VEN) to develop a multifunctional wound dressing membrane for diabetic wound healing. A novel CMC-LIGVEN membrane was prepared by casting and tested for structural, physicochemical, biological, and wound-healing characteristics. Isolation of CEL and LIG was successfully accomplished, and NMR characterization confirmed their structures. The degree of substitution of the prepared CMC was found to be 0.85. Swelling was examined under varying pH levels, with swelling up to 89% occurring at pH 8.5. The membrane displayed remarkable antimicrobial activity against *E. coli* and *S. aureus* at 75 µg/mL. In addition, in vitro anti-inflammatory activity was determined, with an IC₅₀ of 98.2 µg/mL. In vivo experiments for diabetic wound treatment revealed faster wound healing, better epithelialization, and increased angiogenesis in the CMC-LIG-VEN group compared to the povidone-iodine group. Improved blood perfusion and oxygenation were also observed using ultrasound and photoacoustic imaging. Overall, the CMC-LIG-VEN membrane, prepared from sugarcane bagasse, exhibits excellent biocompatibility, antimicrobial and anti-inflammatory effects, and advanced wound-healing properties.

Keywords: Biodegradable, Carboxymethyl Cellulose, Diabetic Wound, Lignin.

Starch-Based CaCO₃ Nanocomposite Hydrogel for Efficient Methylene Blue Adsorption from Aqueous MediumR. Mohanapriya¹, Indra Sulania², E. Kayalvizhy^{1*}¹*Department of Chemistry, PSGR Krishnammal College for Women, Coimbatore, Tamil Nadu, India.*²*Materials Science Division, IUAC, New Delhi, India***Abstract**

Poly (N-cyclohexylacrylamide-co-starch methacrylate) CaCO₃ nanocomposite hydrogels were synthesized by in-situ free-radical copolymerization in DMSO/water medium using potassium persulfate (KPS) as initiator and N, N'-methylenebisacrylamide (MBA) as crosslinker. The prepared hydrogel was investigated for the adsorption of methylene blue (MB) from aqueous solution. Batch adsorption experiments were performed to study the influence of contact time and initial dye concentration on MB removal. The residual dye concentration was determined using UV–Visible spectrophotometry, and the adsorption efficiency was evaluated from the change in dye concentration before and after treatment. The results demonstrate the potential of the starch-based CaCO₃ nanocomposite hydrogel as an effective adsorbent for methylene blue removal from aqueous media. The discharge of synthetic dyes into water bodies is an important environmental concern because of their persistence and resistance to conventional treatment processes. Methylene blue (MB), a cationic dye, is widely used as a model pollutant in adsorption studies. Nanocomposite hydrogels combine the swelling and water-retention properties of crosslinked polymers with the functional characteristics of inorganic nanoparticles. In the present study, a starch-based CaCO₃ nanocomposite hydrogel was investigated as an adsorbent for the removal of MB from aqueous solution. Poly (N-cyclohexylacrylamide-co-starch methacrylate) CaCO₃ nanocomposite hydrogel was prepared by in-situ free-radical copolymerization using KPS and MBA in DMSO/water medium. A known mass of the dried hydrogel was immersed in MB solutions of predetermined concentrations. The adsorption experiments were carried out for different contact times. After treatment, the hydrogel was separated and the residual MB concentration was measured by UV–Visible spectrophotometry. The percentage removal and adsorption capacity were calculated from the initial and residual dye concentrations. The prepared nanocomposite hydrogel exhibited adsorption toward methylene blue from aqueous solution. A decrease in the MB concentration was observed with increasing contact time, indicating progressive uptake of dye molecules by the hydrogel network. The adsorption behavior was also influenced by the initial MB concentration. The three-dimensional porous structure of the swollen hydrogel facilitates diffusion of MB molecules into the polymer network, while the functional groups of the polymer matrix and CaCO₃ nanoparticles may contribute to dye–adsorbent interactions. The obtained results indicate that the starch-based CaCO₃ nanocomposite hydrogel can serve as a potential adsorbent for the removal of MB from aqueous systems. The starch-based CaCO₃ nanocomposite hydrogel was successfully prepared and evaluated for methylene blue adsorption. The hydrogel showed effective interaction with MB and demonstrated its ability to reduce the dye concentration in aqueous solution. The adsorption behavior was influenced by contact time and initial dye concentration. These findings indicate the potential application of the starch-based CaCO₃ nanocomposite hydrogel as an adsorbent for dye-contaminated industrial wastewater treatment.

Keywords: Nanocomposite hydrogel, Starch methacrylate, N-cyclohexylacrylamide, CaCO₃, Methylene blue, Adsorption, Wastewater treatment.

OP-BM- 110

**Computational Studies on Biologically Important MRI Agents - A DFT
Study**

Understanding Nanomaterial Toxicity: Evolution, Mechanisms, and Emerging Tools for Risk Assessment and Sustainable Nanotechnology

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Abstract

Nanotechnology has rapidly transformed several fields, including medicine, agriculture, environmental science, and consumer products, leading to increasing exposure to engineered nanomaterials. Nanotoxicology has therefore emerged as an important field for understanding the potential adverse effects of nanomaterials on human health and the environment. This review presents the evolution of nanotoxicology over the past two decades, highlighting major advances in understanding the biological and environmental interactions of nanomaterials. Early research primarily focused on cellular toxicity and biological responses, whereas recent studies have increasingly investigated molecular mechanisms, environmental fate, and predictive approaches. Nanomaterial toxicity is influenced by several physicochemical characteristics, including particle size, shape, composition, surface properties, dose, and exposure conditions. The review also discusses important mechanisms such as oxidative stress, inflammation, mitochondrial dysfunction, and genotoxicity. Advances in three-dimensional biological models, organoids, and computational approaches have improved the assessment of nanomaterial toxicity. Artificial intelligence and machine learning offer promising tools for predicting toxicity and supporting safer nanomaterial design, although limitations such as heterogeneous datasets, overfitting, and insufficient external validation remain. The review emphasizes the need for standardized testing methods, harmonized datasets, realistic exposure models, and effective regulatory frameworks. Integrating these approaches through safe-by-design strategies can support the development of safer, sustainable, and responsible nanotechnology.

Keywords: Nanotoxicology, Nanomaterial toxicity, Mitochondrial dysfunction, Predictive toxicology, AI in nanotoxicology.

Eggshell Membrane–CeO₂ Nanocomposite as a Biocompatible Platform for Mitigating Toxicity-Induced Redox Imbalance and Organ Damage

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Abstract

Unhydrolyzed eggshell membrane (u-ESM) is a naturally abundant biopolymer rich in protein functional groups. Its biomimetic structure closely resembles the extracellular matrix, making it highly attractive for biomedical applications. In this study, we successfully synthesized cerium oxide (CeO₂)-loaded u-ESM nanocomposites using a solution heating method, producing uniformly dispersed CeO₂ nanoparticles with an average particle size of approximately 25 nm within the heat-treated u-ESM matrix. Extensive physicochemical characterization using FTIR, FESEM, TEM, EDS, XRD, UV-Vis, and XPS analyses confirmed the preservation of biofunctional groups in u-ESM, a mixed Ce³⁺/Ce⁴⁺ redox state, oxygen-vacancy-rich CeO₂, and enhanced surface activity. The uniform nanoscale dispersion and redox activity of CeO₂ impart strong antioxidant and antimicrobial efficacy through efficient reactive oxygen species (ROS) regulation and cellular protection. To the best of our knowledge, this is the first report describing a CeO₂-integrated unhydrolyzed eggshell membrane nanocomposite developed for the dual purpose of toxicity-induced organ protection and sperm cryopreservation. The unique combination of a proteinaceous biomimetic matrix and redox-active nano-CeO₂ provides a multifunctional platform with enhanced bio-interfacial compatibility, antioxidant capacity, and antimicrobial performance. In vivo studies demonstrated that u-ESM/CeO₂ nanocomposite treatment effectively mitigated DDT-induced liver hypertrophy, kidney injury, and testicular degeneration in male Wistar rats. Furthermore, in vitro investigations revealed sustained sperm viability, morphology, and motility under heat-induced stress conditions, highlighting its potential as a protective cryopreservation medium. These findings establish the u-ESM/CeO₂ nanocomposite as a promising biomaterial for antimicrobial intervention, oxidative stress mitigation, fertility preservation, advanced ART, IVF, and regenerative medicine applications.

Keywords: Eggshell membrane, CeO₂ nanoparticles, Male infertility, Cryopreservation

Green Synthesis of Se NPs Using Papaver burseri Leaf Extract and Investigation of Their Anticancer Mechanisms against AGS Cancer cells

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Abstract

AGS Cancer remains a major global health burden and highlights the continuing need for novel, effective, and safer therapeutic strategies. Selenium nanoparticles (SeNPs) have emerged as promising nanomaterials for biomedical applications because of their distinctive physicochemical properties, antioxidant/pro-oxidant behavior, and potential anticancer activity. Green synthesis using plant extracts offers an environmentally friendly and sustainable approach to nanoparticle production, in which naturally occurring phytochemicals can participate in the reduction, stabilization, and surface functionalization of nanoparticles. Papaver burseri is a medicinally important plant containing diverse phytochemicals that may contribute to the biological activity and functionalization of SeNPs. The proposed study aims to develop selenium nanoparticles using Papaver burseri leaf extract through a green synthesis approach and to investigate their physicochemical characteristics and anticancer potential against human gastric cancer cells. The synthesized SeNPs will be optimized and comprehensively characterized using UV–visible spectroscopy, Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), dynamic light scattering (DLS), and zeta-potential analysis. The biological properties of the synthesized SeNPs will be systematically evaluated, including antioxidant, antimicrobial, and anti-inflammatory activities. Selectivity toward cancer cells may be assessed using a suitable normal cell line. To elucidate the underlying anticancer mechanisms, further investigations will examine intracellular reactive oxygen species generation, mitochondrial membrane potential, apoptosis, cell-cycle progression, and selected molecular markers associated with oxidative stress and apoptotic signaling. The study is expected to establish a reproducible and sustainable method for the green synthesis of Papaver burseri-mediated SeNPs and generate comprehensive physicochemical and biological evidence regarding their anticancer potential. The findings may provide a scientific basis for further development of plant-mediated SeNPs as potential nanotherapeutic candidates for AGS cancer and other biomedical applications.

Keywords: Papaver burseri, selenium nanoparticles, antimicrobial activity, anti-inflammatory activity.

**Development and Molecular Evaluation of *Azadirachta indica* - loaded
CeO₂ NPS as a Novel Nanotherapeutic for MCF-7 Cancer Cells**

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Abstract

Breast cancer remains one of the leading causes of cancer-related mortality worldwide, emphasizing the need for safer, effective, and multifunctional therapeutic strategies. Green nanotechnology offers a promising approach for developing biologically active nanoparticles by combining the therapeutic properties of medicinal plants with the unique physicochemical characteristics of metal oxide nanoparticles. *Azadirachta indica*, a medicinal plant rich in alkaloids, diterpenoids, glycosides, flavonoids, phenolics, and other bioactive constituents, possesses reported antioxidant, anti-inflammatory, antimicrobial, and anticancer properties. The present study aims to develop *Azadirachta indica*-mediated cerium oxide nanoparticles (CeO₂ NPs) as a novel nanotherapeutic platform for breast cancer. The synthesized nanoparticles will be characterized using UV–visible spectroscopy, FTIR, XRD, SEM/TEM, EDX, DLS, and zeta-potential analysis to determine their optical properties, functional groups, crystalline structure, morphology, elemental composition, particle-size distribution, and surface charge. The biological potential of the nanoparticles will be systematically evaluated for antimicrobial, antioxidant, and anti-inflammatory activities using appropriate in vitro assays. Their anticancer efficacy will be investigated against selected breast cancer cell lines, with a normal cell line included to assess cytotoxic selectivity. Molecular mechanisms will be explored through analysis of reactive oxygen species generation, mitochondrial membrane-potential alteration, apoptosis, nuclear damage, cell-cycle progression, and expression of key apoptosis- and proliferation-associated markers. Comparative evaluation of *Azadirachta indica* extract and synthesized CeO₂ NPs will help determine the contribution of plant-derived phytochemicals to the observed biological effects. Overall, this study seeks to establish *Azadirachta indica*-mediated CeO₂ NPs as a multifunctional and sustainable nanotherapeutic candidate with potential applications in breast cancer research and biomedical therapy.

Keywords: *Azadirachta indica*; Anticancer activity; Anti-inflammatory activity; Antimicrobial activity; ROS; Nanotherapeutics.

Targeted MoSe₂/ZnO-PEG-cRGD Nanocomposite for Enhanced Wound Healing and Tissue Regeneration

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Abstract

Effective wound management remains a significant therapeutic challenge due to microbial infection, oxidative stress, prolonged inflammation, and impaired cellular regeneration. In the present study, a multifunctional MoSe₂/ZnO-PEG-cRGD nanocomposite was developed as an advanced nanotherapeutic platform for promoting wound healing and tissue regeneration. The nanocomposite was designed by integrating molybdenum diselenide (MoSe₂) and zinc oxide (ZnO) nanoparticles with polyethylene glycol (PEG) and cyclic RGD (cRGD) peptide functionalisation to improve stability, biocompatibility, and cellular interaction at the wound site. The physicochemical characteristics of the developed nanocomposite were investigated using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), dynamic light scattering (DLS), zeta potential analysis, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The wound-healing potential was evaluated through antibacterial, antioxidant, cell viability, cell migration, and in vitro wound closure assays. The MoSe₂/ZnO-PEG-cRGD nanocomposite demonstrated favourable physicochemical properties and enhanced biological activity compared with the individual components. The nanocomposite exhibited significant antibacterial activity against wound-associated bacterial pathogens and showed effective free-radical scavenging activity, suggesting its potential to reduce oxidative stress at the wound site. Furthermore, treatment with the nanocomposite promoted cellular proliferation and migration and accelerated wound closure in vitro. Enhanced cellular interaction associated with cRGD functionalisation further supported the regenerative potential of the nanocomposite. Overall, these findings indicate that MoSe₂/ZnO-PEG-cRGD nanocomposites represent a promising multifunctional nanoplatform for accelerating wound healing by simultaneously addressing microbial infection, oxidative stress, and impaired tissue regeneration. This nanocomposite-based strategy may provide a potential approach for the development of advanced wound-healing materials for effective tissue repair.

Keywords: MoSe₂/ZnO nanocomposite, PEG, cRGD peptide, Wound healing, Antibacterial activity, Antioxidant activity, Cell migration, Tissue regeneration.

Protective effects of *Persea americana* leaf extract–fucoïdan–chitosan–silver nanoparticle complex against oxidative stress in CHO-K1 cells

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Abstract

Polycystic ovary syndrome (PCOS) is a multifactorial endocrine disorder closely associated with oxidative stress, mitochondrial dysfunction, and increased apoptosis in ovarian cells. The present study aimed to evaluate the cytoprotective and antioxidant potential of a novel nanocomposite formulation consisting of *Persea americana* leaf extract combined with Fucoïdan, Chitosan nanoparticles, and Silver nanoparticles in CHO-K1 cells as an in vitro model relevant to ovarian function. The synthesized nanocomplex was assessed for its effects on cell viability, oxidative stress, mitochondrial integrity, and apoptosis using standard biochemical assays. Cell viability was determined using the MTT assay, while intracellular Reactive Oxygen Species levels were measured to evaluate oxidative stress. Mitochondrial function was analysed via Mitochondrial Membrane Potential, and apoptotic changes were quantified using Apoptosis assays. Results demonstrated that treatment with the nanocomplex significantly enhanced cell viability and reduced intracellular ROS levels compared to untreated controls. Furthermore, the formulation preserved mitochondrial membrane potential and decreased apoptotic cell populations, indicating improved cellular health and resistance to oxidative imbalance. These effects may be attributed to the synergistic antioxidant properties of *Persea americana* phytoconstituents and the enhanced bioavailability conferred by the fucoïdan–chitosan–silver nanoparticle delivery system. In conclusion, the developed nanocomposite exhibits promising antioxidant and cytoprotective effects in CHO-K1 cells and may serve as a potential therapeutic strategy for managing oxidative stress-related ovarian dysfunctions such as PCOS. However, further in vivo and mechanistic studies are required to validate its clinical applicability.

Key Words: CHO-K1 cells, Reactive Oxygen Species, Mitochondrial Membrane Potential, Polycystic ovary syndrome (PCOS), Nanocomposite.

Nano-Biosensors for Early Disease Diagnosis: Recent Advances and Biomedical Applications

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Abstract

Nano-biosensors are modern tools used to detect diseases at an early stage. They combine nanomaterials with biological molecules to identify specific disease-related biomarkers. Early diagnosis is important for the effective treatment and prevention of diseases such as cancer, diabetes, cardiovascular diseases, and infectious diseases. Nanomaterials such as gold nanoparticles, graphene, carbon nanotubes, and quantum dots have unique properties that help to improve the sensitivity and accuracy of biosensors. This review focuses on the recent developments and biomedical applications of nano-biosensors in early disease diagnosis. Different types of nano-biosensors, including electrochemical, optical, colorimetric, and fluorescence-based sensors, are discussed. The role of nanomaterials in improving signal detection and identifying specific biomarkers is explained. Their applications in glucose detection, cancer biomarker identification, and infectious disease diagnosis are also highlighted. Nano-biosensors have several advantages, including rapid detection, high sensitivity, small sample requirements, and the possibility of developing portable diagnostic devices. However, challenges such as sensor stability, reproducibility, cost, toxicity, and the need for clinical validation remain important concerns. Recent advances in wearable biosensors, smartphone-based detection, and point-of-care diagnostic devices provide new opportunities for improving healthcare. Overall, nano-biosensors show promising potential in the field of biomedical diagnosis. Further research and development may help in designing reliable, affordable, and user-friendly diagnostic tools for early disease detection and better patient care.

Keywords: Nano-biosensors, Nanomaterials, Early Disease Diagnosis, Biomarkers, Biomedical Applications, Biosensing.

Phytochemical Screening and *In Vivo* Excision Wound Healing Activity of *Hemigraphis Colorata*

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Abstract

Wound healing is a dynamic and complex biological process comprising overlapping phases of inflammation, wound contraction, epithelialization, granulation tissue formation and tissue remodelling. Medicinal plants have long been valued in traditional wound management systems owing to the diverse array of bioactive phytoconstituents they contain. The present study was undertaken to evaluate the phytochemical composition and *in vivo* excision wound healing activity of *Hemigraphis colorata*. Preliminary qualitative phytochemical screening of the plant extract revealed the presence of pharmacologically important constituents such as anthraquinones, flavonoids, steroids, sugars and reducing sugars, indicating its potential therapeutic value. The *in vivo* wound healing efficacy was assessed using an excision wound model in experimental animals, with untreated and extract-treated groups maintained for comparison. Topical application of 10% *Hemigraphis colorata* extract resulted in a significantly faster rate of wound contraction, along with improved re-epithelialization, enhanced granulation tissue formation and better collagen organization compared with the untreated control group. The phytochemicals present in the extract accelerate the wound-healing process by minimizing oxidative tissue damage at the wound site. These findings collectively suggest that *Hemigraphis colorata* possesses significant phytochemical richness and promising wound-healing potential, supporting its traditional use in skin and tissue repair. Further phytochemical and pharmacological investigations are warranted to isolate and characterize the specific active compounds responsible for this activity and to elucidate their underlying mechanism of action.

Keywords: *Hemigraphis colorata*, Phytochemical Screening, *In vivo* Excision Wound Healing, Wound Healing Model.

In Silico Molecular Docking and In Vitro Anticancer Evaluation of Bioactive Constituents from *Trigonella foenum-graecum* Leaves against Human Malignant Cells

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Abstract

Overexpression of the anti-apoptotic protein BCL-2 contributes to resistance to chemotherapy in several solid malignancies. *Trigonella foenum-graecum* (fenugreek) leaves represent an underutilized plant biomass containing diverse secondary metabolites with potential pharmacological activities. To investigate the potential interaction of bioactive constituents identified from aqueous *T. foenum-graecum* leaf extract with human BCL-2 using molecular docking and to evaluate the in vitro cytotoxic activity of the extract against human cancer cell lines. Bioactive constituents identified by GC–MS analysis were subjected to molecular docking studies against the human BCL-2 protein (PDB ID: 2XA0). The in vitro cytotoxic activity of the aqueous leaf extract was evaluated using the MTT assay at concentrations ranging from 18.75 to 300 µg/mL for 24 h against human lung carcinoma (A549) and hepatocellular carcinoma (HepG2) cells. Experiments were performed in triplicate (n = 3), and IC₅₀ values were determined from concentration–response curves. Molecular docking revealed favorable interactions between selected phytoconstituents and the BCL-2 binding region. The sesquiterpenoid derivative, (3R,4aS,8aS)-8a-methyl-5-methylene-3-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,8a-octahydronaphthalene, exhibited a docking score of –6.31 kcal/mol with a predicted inhibition constant (K_i) of 23.53 µM and occupied the hydrophobic BH3-binding groove. Dodecanoic acid ethyl ester showed a docking score of –4.69 kcal/mol and formed hydrogen-bond interactions with HIS120 and ARG129. The MTT assay demonstrated concentration-dependent reduction in cell viability, with IC₅₀ values of 93.39 µg/mL (R² = 0.998) for A549 cells and 86.06 µg/mL (R² = 0.999) for HepG2 cells. The findings demonstrate that the aqueous *T. foenum-graecum* leaf extract exhibits in vitro cytotoxic activity against A549 and HepG2 cells, while its identified phytoconstituents show favorable in silico interactions with BCL-2. These results provide preliminary evidence supporting further investigation of *T. foenum-graecum* leaf-derived bioactives as potential anticancer candidates. Further mechanistic studies, including assessment of BCL-2 expression, apoptotic markers, and mitochondrial pathway activation, are required to establish the proposed mechanism of action.

Keywords: *Trigonella foenum-graecum*; BCL-2; molecular docking; cytotoxicity; A549; HepG2; phytoconstituents; apoptosis.

Valorization of Banana Flower Waste for Green Synthesis of Zinc Oxide Nanoparticles and Development of an Antibacterial Biodegradable Food-Packaging Film

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Abstract

Banana flower is an underutilized agro-food resource that contains valuable bioactive compounds and can be explored for sustainable nanomaterial production. This study aims to valorize banana flower waste through the green synthesis of zinc oxide nanoparticles (ZnO NPs) and their incorporation into a biodegradable food-packaging film with antibacterial activity. Banana flower waste extract will be prepared and used as a green reducing and stabilizing medium for ZnO nanoparticle synthesis. The synthesized nanoparticles will be characterized using suitable physicochemical techniques to evaluate their formation, size, morphology, and functional characteristics. The ZnO NPs will then be incorporated into a biodegradable polymer matrix to develop an active food-packaging film. The prepared film will be evaluated for its physicochemical properties, mechanical characteristics, barrier performance, and antibacterial activity against selected food-associated microorganisms. The proposed approach combines agricultural waste valorization, green nanotechnology, and sustainable packaging in a single platform. The developed ZnO-based biodegradable film is expected to provide antibacterial functionality while reducing dependence on conventional plastic packaging, demonstrating the potential of banana flower waste as a sustainable resource for value-added nanomaterial and food-packaging applications.

Keywords: Banana flower waste, Zinc oxide nanoparticles, Green synthesis, Antibacterial food packaging, Biodegradable film

Green synthesis of Gold Nanoparticles (AuNPs) using *the aqueous extract of Epipremnum aureum* and their antioxidant efficiency

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Abstract

Today, the combination of nanotechnology and biology has created a new essential field called nano-biotechnology which attracts the researchers to adopt green chemistry approaches through nano-phyto technology. Nano sized (1 -100 nm) material has unique properties like optical, electronic, catalytic, biological and pharmacological properties due to their size and shape. The use of extracts of plant parts, micro-organisms and biomass wastes as reducing and stabilizing agents in preparation of metallic nanoparticles has made this method as single stage, quick, nontoxic, and eco-friendly method over hazardous chemical and physical methods. Gold is known for its biomedical applications since from ancient period. World Health Organization (WHO), recently reports us that 90% of the global population rely on metal mixed (particularly gold) herbal medicines for their cosmetic and health care ailments. In this study gold nanoparticles (NPs) are synthesized using aqueous extract of *Epipremnum aureum* (commonly known as money plant/marble queen/silver vine/hunters rope/ivy arum belongs to Araceae family). The biosynthesized gold nano particles (AuNPs) are characterized by the spectral studies UV visible, FT-IR for the NPs formation, presence of bio functional groups and their antioxidant potentials are assessed by standard assay method.

Keywords: gold nanoparticles, money plant extract, UV Visible, FTIR, antioxidant potentials.

**Synthesis, Characterization and Antimicrobial Evaluation of a
4-Nitroaniline-2,4-Imidazolidinedione-Formaldehyde Terpolymer and its
Ni(II) Polychelate**

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Abstract

A new terpolymer resin (NAHF) was synthesized via condensation polymerization of 4-nitroaniline, 2,4-imidazolidinedione and formaldehyde (1:1:2) in dimethylformamide and used as a polymeric ligand to prepare its Ni(II) polychelate. Both compounds were characterized by elemental analysis, FT-IR, UV-Visible and NMR (^1H & ^{13}C) spectroscopy, with molecular weights determined by gel permeation chromatography. Antimicrobial activity, assessed by the disc diffusion method ($100\ \mu\text{g mL}^{-1}$), showed inhibition zones of 7 mm (*S. aureus*) and 6 mm (*E. coli*) for NAHF, versus 10 mm and 8 mm for the polychelate, which was additionally active against *C. albicans* (9 mm). Enhanced activity upon chelation reflects reduced polarity at the metal centre, favouring membrane permeation and supporting NAHF-Ni(II) as a candidate antimicrobial polymer.

Keywords: 2,4-Imidazolidinedione, Polycondensation, Antimicrobial Evaluation, GPC

Understanding The Chemistry of Amygdalin – A Computational Approach

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Abstract

Amygdalin {IUPAC name [(6-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy][phenyl acetonitrile]}}, was isolated for the first time in the 19th century in 1830. Amygdalin is a naturally occurring cyanogenetic glucoside found in the kernels or seeds of Rosaceae (almond, apple, apricot, chury, peach, pear, plum, quince). Amygdalin is called interchangeably vitamin B17 or Laetrile. Since more than a hundred years, there has been reports about its unique anticancer properties. In 1845 it was used to treat cancer in Russia. Then it has been practiced as an anticancer agent in many countries especially Mexico. The positive influence of amygdalin on many diseases like: bladder cancer, prostate cancer, cervical cancer, colon cancer, dromyelocytic leukemia, chronic kidney disease, psoriasis and others are tested and reported by many groups. Though the amygdaline is referred as laetrile, amygdalin is not structurally synonymous with laetrile. Biological studies are known for amygdalin but the interactions of amygdalin with biomolecules at molecular level are sparse. Computational studies on molecules are being routinely used to address the chemical problems with good accuracy. We have studied the structural features of the amygalin at molecular level using computational chemistry methods, like Density Functional Theory (DFT) methods. The presence of cyanide group in the amygdalin molecule is the crucial factor for acceptance or negligence of this biologically important, naturally occurring compound. Our studies shed light on this aspect in specific by using computational chemistry tools. Key words: Amygdalin, cyanogenetic glucoside, vitamin B17 or Laetrile, seeds of Rosaceae, anticancer agent, bladder cancer, prostate cancer, cervical cancer, colon cancer, dromyelocytic leukemia, chronic kidney disease, psoriasis, DFT.

DES/Biotin-g-Lysine-PEG Polymeric Micelles for Targeted and pH-Responsive Anticancer Drug Delivery

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Abstract

Cancer chemotherapy is often limited by poor selectivity of anticancer drugs toward tumor cells, resulting in damage to healthy tissues and undesirable systemic side effects. This study focuses on the development of a targeted polymeric nanocarrier for controlled anticancer drug delivery using a deep eutectic solvent (DES) and biotin-g-lysine-co-polyethylene glycol (PEG). Deep eutectic solvents were prepared using cetrimonium bromide (CTAB) and lactic acid, while biotin-g-lysine-co-PEG was developed as a targeting polymeric carrier. The DES/polymeric micelles were designed to encapsulate the anticancer drugs paclitaxel (PTX) and 7-hydroxycoumarin (7-HC). The synthesized carrier and drug-loaded micelles were characterized using spectroscopic, thermal and morphological techniques including FTIR, NMR, XRD, Raman, TGA, AFM, SEM and TEM. Drug loading and in-vitro release were investigated using UV spectrophotometry and dialysis methods at different pH conditions. The study demonstrated successful formation of the DES/biotin-g-lysine-PEG polymeric micelles and successful encapsulation of PTX and 7-HC. FTIR analysis supported hydrogen-bonding interactions, while SEM, TEM and AFM confirmed the morphology of the micelles. Importantly, drug-release behavior was found to be pH dependent at pH 2.8, 5.5 and 6.8. The biotin-functionalized polymeric micelle system therefore provides a potential platform for controlled and targeted anticancer drug delivery, with scope for further evaluation using cancer cell-line studies.

Keywords: Cancer therapy; Nanocarrier; Deep eutectic solvent; Biotin; PEG; Polymeric micelle; Paclitaxel; 7Hydroxycoumarin; Targeted drug delivery; pH-responsive drug release.

New generation Dressing: TCP/PCL Nanofibres for Wound Healing Application

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Abstract

Wound healing remains a significant clinical challenge, particularly in chronic and complex wounds where delayed tissue regeneration, infection, excessive inflammation, and inadequate extracellular matrix formation hinder the healing process. Electrospun nanofibrous scaffolds have emerged as promising wound dressing materials because their highly porous and interconnected architecture closely mimics the fibrous structure of the native extracellular matrix (ECM), thereby supporting cellular attachment, proliferation, migration, and tissue regeneration. In this study, tricalcium phosphate (TCP)-infused polycaprolactone (PCL) nanofibres are proposed as a bioactive composite scaffold for wound healing applications. PCL was selected owing to its biocompatibility, biodegradability, favourable mechanical properties, and ability to form continuous nanofibres through electrospinning. However, its hydrophobic nature and relatively limited bioactivity may restrict cellular interactions. The incorporation of TCP, a calcium phosphate-based bioactive ceramic, is therefore intended to enhance the surface bioactivity, hydrophilicity, and biological performance of the PCL nanofibrous matrix. TCP particles are uniformly dispersed within the PCL solution and fabricated into composite nanofibres using the electrospinning technique. The resulting fibrous scaffolds can be characterized using scanning electron microscopy to evaluate fibre morphology, diameter, and surface characteristics, while Fourier-transform infrared spectroscopy and X-ray diffraction can confirm the incorporation and interaction of PCL and TCP phases. The incorporation of TCP is expected to modify the physicochemical properties of the PCL nanofibres and provide biologically relevant calcium and phosphate ions during interaction with the physiological environment. These ions may contribute to improved cellular responses and support the regeneration process. Furthermore, the high surface-area-to-volume ratio and porous structure of the electrospun scaffold may facilitate gaseous exchange and fluid management while providing a favourable microenvironment for wound-site cells. The wound healing potential of TCP-infused PCL nanofibres can be evaluated through *in vitro* biocompatibility, cell adhesion, proliferation, and cell migration studies, together with assessment of the scaffold's wettability, degradation behaviour, and mechanical properties. The developed composite is anticipated to exhibit enhanced cellular compatibility compared with pristine PCL while maintaining sufficient structural integrity during the healing period. Overall, the integration of bioactive TCP into electrospun PCL nanofibres offers a promising strategy for developing multifunctional wound dressing scaffolds with ECM-mimicking morphology, improved bioactivity, and favourable tissue interaction. This work may contribute to the advancement of next-generation biodegradable nanofibrous materials for skin tissue regeneration and wound healing applications.

Key words: TCP, PCL Nanofibres, wound healing, Electrospinning

Unveiling the Biocompatibility of Biosynthesized CeO₂ NPs Incorporated HAp/PVA and Dye Degradation Applications

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Abstract

The development of multifunctional biomaterials with simultaneous biomedical and environmental remediation capabilities has attracted considerable attention in recent years. In the present study, cerium oxide nanoparticles (CeO₂ NPs) were biosynthesized using Rosary Pea leaf extract and subsequently incorporated into a hydroxyapatite (HAp) by the ultrasonic assisted wet chemical precipitation method, finally CeO₂ NPs incorporated HAp powder was infused into the PVA polymer matrix. The study aims to decode the influence of biosynthesized CeO₂ NPs on the structural, physicochemical, biocompatibility, and photocatalytic properties of the developed composite. Hydroxyapatite provides excellent chemical similarity to the mineral phase of natural bone, osteoconductive properties, and bioactivity, whereas PVA contributes flexibility, film-forming ability, and improved processability. The incorporation of CeO₂ NPs is expected to introduce enhanced surface reactivity and redox activity associated with the reversible Ce³⁺/Ce⁴⁺ transition and oxygen-vacancy-mediated mechanisms. The biosynthesized CeO₂ NPs and CeO₂-incorporated HAp/PVA composites can be systematically characterized using X-ray diffraction, Fourier-transform infrared spectroscopy, UV–visible diffuse reflectance spectroscopy, electron microscopy, and elemental analysis to evaluate phase formation, functional-group interactions, optical properties, morphology, and elemental distribution. The optical response and band-gap characteristics of CeO₂ are further correlated with its photocatalytic performance. Biocompatibility can be assessed through in vitro cytocompatibility studies, including cell viability, cellular morphology, and live/dead staining, to understand the interaction between the composite surface and biological cells. The results are expected to reveal whether the incorporation of an optimized concentration of biosynthesized CeO₂ NPs improves cellular compatibility while maintaining the bioactive characteristics of the HAp/PVA matrix. In addition to its biomedical potential, the multifunctionality of the composite is explored through the degradation of an organic dye under suitable light irradiation. The reduction in the characteristic UV–visible absorption intensity of the dye, Rhodamine B is used to monitor photocatalytic degradation and evaluate the role of CeO₂-induced charge separation and reactive oxygen species generation. Thus, this work establishes a sustainable approach for integrating green-synthesized functional nanoparticles into a bioactive polymer–ceramic matrix. The findings are anticipated to provide valuable insights into the relationship between nanoparticle incorporation, biocompatibility, and photocatalytic activity, highlighting CeO₂–HAp/PVA composites as promising multifunctional materials for future biomedical and environmental applications.

Keywords: Ceriumoxide nanoparticles, Hydroxyapatite, Polyvinylalcohol, Biocompatibillity, Dye degradation

**Growth and Characterization of Glycine-Based Nonlinear Optical
Materials for Biomedical Applications**

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Abstract

This project focuses on the synthesis and characterization of glycine-based semi-organic nonlinear optical (NLO) crystals, which may be relevant to biomedical applications. A hybrid crystal with improved optical and structural features was formed by combining glycine, an amino acid, with an appropriate inorganic component. The slow evaporation method was used to synthesize the crystals under carefully regulated temperature and solution conditions. Powder XRD was used to examine the structural properties, and Fourier-transform infrared spectroscopy was used to examine functional-group interactions. Optical transparency and absorption edge were assessed using UV–visible spectroscopy. Thermal stability was determined through thermogravimetric and differential thermal analyses. The dielectric properties and microhardness were studied to check how stable the crystal is in real-world use. The nonlinear optical behavior was examined using a second-harmonic generation test. The crystal is made with a material that has a good optical response and can be used in small photonic devices. This glycine-based semi-organic crystal has promise for use in optical sensing, bioimaging, diagnostic tools, and other nonlinear-photonic uses. More tests are needed on biocompatibility, how it affects cells, and how it works in devices.

Keywords: Glycine; semi-organic crystal; nonlinear optics; single-crystal growth; SHG; optical characterization; biomedical photonics.

The Glymphatic System as an Emerging Therapeutic Target: Implications for Neurological Disorders and CNS Drug Delivery

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Abstract

The glymphatic system is an emerging brain-wide pathway involved in the movement of cerebrospinal fluid and interstitial fluid and the clearance of metabolic waste from the central nervous system. Increasing evidence has linked alterations in glymphatic function with the accumulation of pathological proteins and neurological disorders, including Alzheimer's disease, Parkinson's disease, stroke, and traumatic brain injury. This review summarizes the current understanding of glymphatic organization and function, with emphasis on astrocytic aquaporin-4, sleep-associated regulation, aging, and meningeal lymphatic drainage. The potential relationship between impaired glymphatic clearance and neurological disease is also examined. In addition, emerging therapeutic approaches aimed at modulating glymphatic and meningeal lymphatic pathways are discussed, with particular attention to their potential relevance to central nervous system drug delivery. Although the field has expanded considerably, important challenges remain in defining the underlying mechanisms, developing reliable methods for assessing glymphatic function in humans, and translating preclinical findings into clinical applications. Understanding these pathways may provide new opportunities for neurological therapeutics and innovative approaches to CNS drug delivery.

Keywords: Glymphatic system, Aquaporin-4, CNS drug delivery, Neurodegeneration, Neurological disorders, Meningeal lymphatics.

Nano-Enabled Multiplex Biomarker Strategy for Early Detection of Colorectal Cancer

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Abstract

Colorectal cancer (CRC) is a major health concern, and early detection is essential for improving clinical outcomes. Conventional screening approaches may have limitations related to invasiveness, accessibility, and the detection of early-stage disease. Recent studies have identified several blood-based biomarkers, including DNA methylation markers, circulating tumour DNA, microRNAs, and protein tumour markers, with promising diagnostic potential. However, individual biomarkers may not provide sufficient information across diverse patient populations. This work proposes a literature-supported nano-enabled multiplex biomarker strategy for the early detection of CRC by integrating complementary biomarker types with nanotechnology-based detection approaches. Published studies have demonstrated the potential of magnetic nanoparticles, plasmonic nanostructures, silicon nanowires, and other nanoscale platforms for sensitive biomarker capture and detection. Based on these findings, a conceptual framework is proposed in which minimally invasive blood samples are analysed for multiple complementary CRC biomarkers using suitable recognition elements and nano-enabled signal generation. The proposed strategy aims to provide a more comprehensive molecular profile than single-biomarker detection and may support the development of rapid and minimally invasive diagnostic approaches. Further experimental development, analytical validation, and large-scale clinical studies will be required to establish the sensitivity, specificity, reproducibility, and clinical applicability of the proposed framework.

Keywords: Colorectal cancer; Early detection; Multiplex biomarkers; Nanotechnology; Nano-enabled biosensing; Liquid biopsy; DNA methylation; Circulating tumour DNA; MicroRNAs; Protein biomarkers.

Fabrication of Biocomposite for Bone Tissue Engineering Applications

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Abstract

The goal of this work is to create a biogenic biocomposite for use in bone tissue engineering. Collagen is also made from fish shells using the alkali extraction method, while hydroxyapatite is extracted from a calcium-rich biowaste source, eggshell, using the wet precipitation process. X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and scanning electron microscopy-energy dispersive X-ray analysis (SEM-EDAX) are used to assess the crystallinity, functional group, morphology, and elemental analysis of the as-prepared biocomposite. Vicker's Hardness and the disk diffusion method are also used to measure mechanical strength and antibacterial activity. Therefore, it is anticipated that biocomposite will enhance the biocompatibility of scaffolds for possible uses in bone tissue engineering.

Keywords: Biogenic, hydroxyapatite, collagen, fish shell and eggshell.

A Study of Biological Properties of Biogenic Derived Composite for Biomedical Applications

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Abstract

Among titanium and its alloys are bone-bonding and biocompatible, they have drawn a lot of interest among metallic implants. The goal is to create a biocomposite coating for metallic implants with superior biological qualities. The duplex layer will be deposited on the metallic implants using the electrodeposition technique. X-ray diffraction, scanning electron microscopy, and Fourier transform infrared spectroscopy were used to analyze the coating. The hydroxyapatite covering as it was created displayed a well-crystallized apatite structure and a compact shape. This coating may increase the mechanical properties of the biocomposite-coated implants by strengthening the adhesion and slowing the substrate's rate of corrosion in a bodily fluid solution. Therefore, biocomposite coating will enhance the metallic implants' mechanical, biocompatible, and corrosion resistance, potentially making them suitable for orthopedic applications.

Keywords: Bioceramic, coating, biomedical applications

Synthesis of Biocomposite for Bone Tissue Engineering Applications

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Abstract

Among hydroxyapatite (HAp)-based bioceramics share chemical similarities with the inorganic components of biological hard tissue, they have the potential to be significant materials. In comparison to commercially manufactured HAp, HAp derived from natural sources is readily available, safe, bioactive, and readily binds with natural bone. Numerous approaches have been explored and developed for the synthesis of HAp. The calcium sources from freshwater sea shells are used in this work to create HAp. The as-synthesized biosamples were characterized by X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), and young's modulus are used to assess the physicochemical, antibacterial, and mechanical strength of the synthesis of HAp and L. aspera composite.

Key word: Bioceramic, Synthesis, antibacterial, biomedical applications.

Synergistic Zirconium-Gallium Co-Doped Chitosan Nanocomposite Scaffolds for Dual-Action Bone Tissue Regeneration and Infection Control

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Abstract

Bacterial infections and slow osteogenesis remain critical challenges in orthopedic implant integration and bone defect repair. This study reports the novel synthesis and characterization of a ternary composite scaffold composed of chitosan bio-polymer co-doped with zirconium (Zr^{4+}) and gallium (Ga^{3+}) ions for multifunctional bone tissue engineering applications. Chitosan serves as a bio-active matrix facilitating cell attachment and biocompatibility, while Zr^{4+} integration enhances mechanical integrity, bio-mineralization, and structural stability. Concurrently, Ga^{3+} ions provide strong broad-spectrum antibacterial activity by disrupting iron metabolism in opportunistic pathogens without inducing cytotoxicity to human osteoblasts. Physical-chemical characterization via FTIR, XRD, and FE-SEM confirms the successful chelation of both metallic species within the chitosan network, yielding a highly porous, interconnected micro-architecture favorable for cell infiltration and nutrient transport. In vitro bio-mineralization assays in simulated body fluid (SBF) demonstrate rapid apatite formation, confirming enhanced osteo-inductivity. Antimicrobial evaluations against *Staphylococcus aureus* and *Pseudomonas aeruginosa* display significant inhibition zones due to the synergistic action of chitosan's membrane disruption and gallium release. Furthermore, cytocompatibility assays with human osteosarcoma cells (MG-63) confirm sustained cell proliferation and elevated alkaline phosphatase (ALP) activity over 14 days. These findings demonstrate that the Zr-Ga-Chitosan ternary composite is a highly promising candidate for orthopedic graft materials and antibacterial bone tissue scaffolds.

Keywords: Chitosan nanocomposites, Zirconium, Gallium, Antibacterial bone scaffolds, Tissue engineering, Dual-doped bio-polymers.

Fabrication and Characterization of an Ethyl Cellulose/Chitosan/PVA– ZrO₂ Porous Scaffold for Tissue Engineering

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Abstract

Tissue engineering plays an important role in the field of bio-medical applications. The bio mimetic scaffold is considered as one of the highly promising materials in tissue engineering as it closely replicates the natural extracellular matrix and supports effective tissue regeneration. In this research work, an ethyl cellulose-based scaffold containing chitosan (CH) and polyvinyl alcohol (PVA), and loaded with zirconium oxide nanoparticles (nano-ZrO₂), was developed using the salt-leaching process. The developed scaffolds were characterised by FT-IR Spectroscopy, Scanning Electron Microscopy (SEM), X-ray Diffraction method (XRD). The degradation tests were examined using phosphate buffer saline solution. The porosity of the scaffold was analysed by using aqueous Ethanol solution. Further, the biological characteristics of the prepared scaffold was analysed using in vitro MTT Assay by vero cells and antibacterial activities was examined by the bacterial species *Staphylococcus aureus* and *Escherichia coli*. Hence, the scaffold developed in this study shows great potential as a viable candidate for tissue engineering, meeting the essential functional requirements.

Key Words: Salt Leaching, Ethyl Cellulose, Porous Scaffold, Degradation, MTT Assay

Development of a Novel Jujube Seed-Based Synbiotic Formulation for the Management of Irritable Bowel Syndrome (IBS)

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Abstract

Irritable bowel syndrome (IBS) is a prevalent gastrointestinal disorder characterized by gut microbial dysbiosis, chronic low-grade mucosal inflammation and a compromised epithelial barrier. While current pharmaceutical interventions primarily provide temporary symptomatic relief, targeting the gut-brain axis through synbiotics offers a sustainable, mechanistically driven therapeutic alternative. Concurrently, agricultural processing generates immense volumes of jujube seeds (*Ziziphus jujuba*), which are frequently discarded as waste despite containing dense concentrations of functional polysaccharides and bioactive flavonoids like spinosin. Research project aims to establish a high-value waste-to-wealth strategy by developing a novel, microencapsulated synbiotic formulation optimized for IBS management. The study utilizes green chemistry extraction techniques to isolate and structurally characterize prebiotic oligosaccharides and polysaccharides from raw jujube seeds. *In vitro* fermentation kinetics will be evaluated using automated co-culture models to screen for synergistic pairing with beneficial *Lactobacillus* and *Bifidobacterium* strains, specifically monitoring short-chain fatty acid (SCFA) production. Furthermore, the optimal prebiotic-probiotic matrix will be microencapsulated to survive simulated gastric transit and achieve targeted colonic release. Finally, *in vivo* therapeutic efficacy will be validated in a pre-clinical IBS mouse model by quantifying shifts in microbial taxonomy via 16S rRNA sequencing, assessing the reduction of pro-inflammatory cytokines and evaluating the restoration of intestinal tight-junction proteins (*claudin-1* and *occludin*). Ultimately, this research bridges agricultural byproduct valorization with clinical nutrition, delivering a scientifically validated, shelf-stable functional supplement that addresses the root causes of chronic IBS.

Harnessing of *labeo catla* fish bones -hydroxyapatite/microcrystalline cellulose for biomedical applications

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Abstract

Human bones consist of an organic and inorganic matrix composed of collagenous fibers embedded with bioceramic material. Hydroxyapatite (HAP) is a bioceramic material whose chemical composition resembles natural hard tissue, exhibiting excellent biocompatibility and bioactivity. To further improve mechanical strength, biopolymers are frequently composited with HAP. In the present work, HAP, was derived from *Labeo catla* waste materials and composited with microcrystalline cellulose (MCC) isolated from naturally abundant banana rachis. The biopolymer possesses an abundant side-chain network of phenolic and aliphatic hydroxyl groups, enabling potential chemical bonding between the hydroxyl groups and calcium ions in the HAP/MCC composite. The synthesized HAP/MCC composite was characterized using Fourier Transform Infrared Spectroscopy (FTIR), X-Ray Diffraction (XRD), and Scanning Electron Microscopy (SEM). Additionally, the mechanical strength of both the synthesized HAP and the HAP/MCC composite was evaluated using Vickers microhardness testing. The results indicate that the HAP/MCC composite is a promising candidate for biomedical applications.

Keywords: *bio ceramic, banana rachis, labeo catla, biopolymer.*

Fluoride Exposure and Female Fertility: A Pilot Study

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Abstract

Fluoride exposure through drinking water may influence female reproductive health by affecting endocrine regulation, oxidative balance, and ovarian function. This pilot cross-sectional study evaluated the association between fluoride exposure and reproductive health among healthy women aged **18–25 years** residing in ten villages of the Palar River bank belt of the erstwhile Vellore District, Tamil Nadu, India, now comprising Vellore, Tirupattur, and Ranipet districts. Women were screened for eligibility, and those with diabetes mellitus, chronic kidney disease, endocrine disorders, pregnancy, vitamin D or calcium supplementation, medication affecting reproductive or mineral metabolism, or incomplete information were excluded. Eligible participants provided drinking-water, blood, and morning spot urine samples for fluoride estimation. Female reproductive hormones and selected biochemical biomarkers were assessed using established methods. Descriptive, correlation, and regression analyses were performed, with statistical significance set at $p < 0.05$. The study aims to characterize fluoride exposure and explore its potential relationship with female reproductive health in this population.

Keywords: Fluoride exposure; Female reproductive health; Palar River; Vellore District; Drinking water; Reproductive hormones; Oxidative stress;

Lead and Arsenic Toxicity and Renal Reabsorption: A Pilot Study

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Abstract

Exposure to toxic metals such as lead and arsenic through contaminated drinking water may impair renal tubular function and disturb the reabsorption of essential electrolytes. This pilot cross-sectional study evaluated the association between lead and arsenic exposure and renal reabsorption biomarkers among healthy adults residing in villages of the Palar River bank belt of the erstwhile Vellore District, Tamil Nadu, India. Participants were screened for eligibility, and demographic, dietary, drinking-water, and medical-history information was collected. Drinking-water, serum, and morning spot urine samples were obtained for estimation of lead, arsenic, and selected biochemical parameters. Renal function was assessed by measuring serum urea, creatinine, electrolytes, and urinary excretion of relevant analytes. The study focused on potential alterations in renal tubular reabsorption associated with lead and arsenic exposure. Descriptive and correlation analyses were performed to evaluate relationships between metal concentrations and renal biomarkers. The findings may provide preliminary evidence of metal-associated renal disturbances in this environmentally exposed population.

Keywords: Lead; Arsenic; Metal toxicity; Renal reabsorption; Renal tubular function; Electrolyte homeostasis; Urinary biomarkers

A Pilot Study on Fluoride Exposure and Male Fertility in the Palar River Belt, Tamil Nadu

G Hepsipa & Dr. R Parameswari*

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Abstract

Fluoride exposure through drinking water may affect reproductive health by disturbing endocrine regulation, oxidative balance, and testicular function. This cross-sectional study evaluated the association between fluoride exposure and male reproductive health among healthy men aged 25–35 years residing in ten villages of the Palar River bank belt of the erstwhile Vellore District, Tamil Nadu, India, now comprising Vellore, Tirupattur, and Ranipet districts. Of 120 men screened, 95 were excluded because of diabetes mellitus, chronic kidney disease, vitamin D or calcium supplementation, medications affecting mineral metabolism, other systemic disorders, or incomplete information. Twenty-five eligible participants were included. Drinking-water, serum, and morning spot urine samples were collected for fluoride estimation. Semen samples were evaluated for sperm concentration, motility, morphology, and viability. Reproductive hormones and oxidative stress biomarkers were also assessed using established biochemical methods. Descriptive, correlation, and regression analyses were performed, with significance set at $p < 0.05$. The study evaluates the relationship between fluoride exposure and male reproductive biomarkers in this population.

Keywords: Fluoride exposure; Palar River; Male fertility; Semen quality; Oxidative stress; Drinking water; Vellore District.

Hesperidin-Functionalized Hydroxyapatite–Bentonite Nanocomposite for Antibacterial and Osteogenic Applications in Bone Regeneration

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Abstract

Bone defects caused by trauma, tumour resection, osteoporosis, or infection often exceed the intrinsic regenerative capacity of bone and are frequently complicated by bacterial colonisation. To address this challenge, we developed a multifunctional nanocomposite scaffold based on hesperidin-functionalised hydroxyapatite–bentonite (Hes@HA-Bent) for simultaneous bone regeneration and antibacterial protection. The HA-Bent matrix was synthesised by *in situ* wet-chemical co-precipitation, followed by hesperidin loading at five concentrations. Hes4@HA-Bent containing 16 wt% hesperidin was identified as the optimised formulation. FTIR and XRD confirmed preservation of the hydroxyapatite phase and bentonite layered structure, together with successful hesperidin incorporation. FE-SEM and EDX demonstrated a nano-rough, porous morphology and homogeneous distribution of Ca, P, O, Si, Al, and C, with a Ca/P ratio close to 1.67. Hesperidin functionalisation improved compressive strength to 63.0 ± 3.5 MPa and compressive modulus to 1420 ± 70 MPa. In MC3T3-E1 pre-osteoblasts, Hes4@HA-Bent maintained >110% cell viability, enhanced proliferation, increased alkaline phosphatase activity by 2.06-fold, promoted mineralised matrix formation by 2.95-fold, and achieved $95 \pm 4\%$ scratch-wound closure at 48 h. Against *Staphylococcus aureus*, the nanocomposite reduced bacterial viability to $3 \pm 2\%$ by day 14, showing activity comparable to vancomycin. These findings demonstrate that Hes4@HA-Bent integrates nanostructured architecture, mechanical competence, osteogenic stimulation, and antibacterial performance, highlighting its potential as a nanotechnology-based biomaterial for infected and non-healing bone defects.

Keywords: Hesperidin; hydroxyapatite; bentonite; nanocomposite; bone regeneration; antibacterial; osteogenesis

Synthesis, Characterization and Enhanced Antimicrobial Activity of Silver Nano dendrite -Decorated Polythiophene Nanocomposite

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Abstract

The development of effective antimicrobial nanomaterials has gained considerable attention owing to the increasing prevalence of microbial contamination and resistance to conventional antimicrobial agents. In the present study, a silver nanodendrite-decorated polythiophene (AgND/PTh) nanocomposite was developed as a multifunctional antimicrobial material. Polythiophene was employed as a conductive polymeric matrix, while silver nanodendrites were incorporated onto its surface to provide a high surface area and abundant active sites for enhanced interaction with microbial cells. The synthesized nanocomposite was systematically characterized using suitable structural, morphological and spectroscopic techniques to investigate its composition, surface morphology, crystallinity and interfacial interactions. The dendritic architecture of silver and its intimate association with the polythiophene matrix are expected to facilitate improved surface activity and synergistic antimicrobial performance. The antimicrobial efficacy of the nanocomposite was evaluated against representative Gram-positive and Gram-negative bacterial strains, and the results demonstrated significant inhibition of microbial growth compared with the individual components. The enhanced activity can be attributed to the combined effects of silver-ion release, generation of reactive oxygen species, membrane disruption and the interaction of the nanocomposite surface with microbial cells. The polythiophene matrix may further contribute to improved dispersion, stability and accessibility of silver nanostructures. The findings highlight the potential of AgND/PTh nanocomposites as promising antimicrobial materials for applications in protective coatings, healthcare-related surfaces, environmental remediation and other areas requiring effective microbial control. This work provides a useful platform for designing polymer-metal nanocomposites with tunable surface properties and enhanced antimicrobial functionality.

Microalgae: An Emerging Approach for Microplastic Bioremediation and Bioplastic Upcycling

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Abstract

The global production of plastic has surged dramatically encompass a range of types including polyethylene (PE), polypropylene (PP), polyvinyl chloride (PVC), polystyrene (PS) and polyester. The deposition of microplastic particles posing a significant threat to aquatic life includes development of toxicity, neurotoxicity, reproductive toxicity, immunotoxicity and phytotoxicity. Wherever microalgae are capable of thriving on abundant waste resources and exhibiting substantial lipid accumulation which represent a more favourable option as biomass source for bioplastic production as they do not compete with food sources. The global scale of plastic pollution is alarming, with millions of tons. Their ability to interact with microplastics through multiple mechanisms, combined with their rapid growth and adaptability, makes them suitable for large-scale applications. Moreover, algal biomass generated during the remediation process can be utilized to produce valuable products. Herein we are addressing the current bioremediation potential of microalgae, pollutant induced bioaccumulation of microplastics and sustainable remediation strategies in removing microplastics and nanoplastics from waste aquatic systems for environmental sustainability (SDGs) and cost effectiveness. In addition to adsorption and aggregation, microalgae secrete extracellular polymeric substances (EPS) and degradative enzymes such as esterases, lipases and laccases, which collectively enhance microplastic removal by facilitating close contact and enabling enzymatic depolymerization of polymer chains. Hydrophobic cyanobacteria cells (HCC) are surface-modified or naturally hydrophobic cyanobacteria that enhance microplastic adsorption, they can self-aggregate and achieve auto-sedimentation. The produced limonene aids in the partial dissolution or softening of microplastics, improves their separation from algal biomass, and promotes overall biodegradation efficiency while remaining environmentally friendly.

Keywords: Microalgae, Microplastic Bioremediation, Bioplastic Upcycling, Circular Bioeconomy.

PP-BM-04

Potentially Bioactive New Cu(II) Complexes: Synthesis, Spectroscopic, Physico-Chemical Investigations, Antibacterial and Radical Scavenging Properties

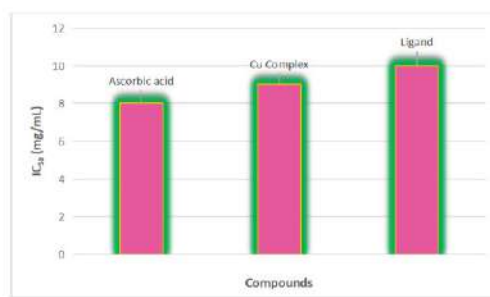
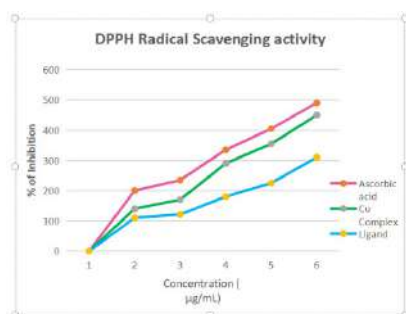
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Abstract

The mononuclear Schiff base Cu(II) complex have been synthesized from the condensation of o-phenylenediamine and 2-acetyl-5-bromothiophene in ethanol. The metal complex have been fully characterized with the help of analytical, conductivity, IR, electronic, and $^1\text{H-NMR}$ studies. The molar conductance value indicates that the complex is non-electrolyte in nature. The IR spectra of synthesized compounds confirmed the coordination of ligand to the metal ion. The UV-Vis and magnetic moment data of the complex suggest a distorted octahedral geometry. The antibacterial activities of the synthesized Cu(II) compound and the Schiff base ligand were tested in vitro against the sensitive organisms *Staphylococcus aureus*, *Bacillus subtilis* as Gram positive bacteria, *Escherichia coli* and *Klebsilla pneumonia* as Gram negative bacteria, and the results are discussed. We found that the antioxidant activity of the Cu(II) complex on DPPH is concentration dependent and the values are higher than that of the Schiff base ligand. The antioxidant activity of the complex was also investigated through the scavenging effect on DPPH.



DPPH Radical Scavenging activity of Ligand **DPPH Scavenging capacities (IC₅₀ (mg/mL) values)**

Keywords: Scavenging effect, Antibacterial assay, o-phenylenediamine.

In Silico and Experimental Evaluation of *Boswellia Serrata* Extract Coatings for Antimicrobial Modification of Melt-Blown Mask Layers

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Abstract

Face mask's melt blown layer has excellent air filtration, yet it has two key limitations, inability to neutralize pathogens and increasing breathability resistance during prolonged use. This study explores this limitation by modification of melt blown layer with *Boswellia serrata* extract. The aim is to develop a biocidal respiratory interface can disinfect while being used. In the present study *Boswellia serrata* resin extract is incorporated into the melt blown material via dip coating technique. This coating-maintained breathability of the material as well. However, uniform surface roughness to the melt-blow fibers, (FESEM), distribution of the phytochemical coating across the material surface (EDX) and integration of oxygen rich functional groups (FTIR). The modified layers exhibited potent contact killing activity against pathogens like *C. albicans*, *S. aureus*, *K. pneumoniae*, and *E. aerogenes*. Thus, study confirmed the transition of melt-blown from a passive filtration to active biocidal system using *Boswellia serrata* resin extract¹⁻⁵.

Keywords: Melt blown; Surface modification; *Boswellia serrata*; Breathability; Facemask

**Green-Synthesized Silver Nanoparticle-Loaded Biopolymer Film:
Preliminary Formulation Screening Using Formulation AI and In Vitro
Characterization**

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Abstract

The traditional wound dressing systems usually offer only passive wound covering that may suffer from certain drawbacks, like inability to provide proper antimicrobial activity, lack of moisture regulation capability etc. Consequently, the aim of the current project is to design and optimize a multi-functional multiscaffold wound-healing film containing silver nanoparticles (AgNPs), chitosan, flaxseed mucilage and polyvinyl alcohol (PVA). The AgNPs are obtained by means of a green, biopolymer-assisted synthesis, with chitosan acting as a matrix for stabilization of nanoparticles and ascorbic acid being used as a reducing agent, followed by the crosslinking of obtained polymeric matrix with the use of sodium tripolyphosphate (TPP). Preliminary characterization of synthesized AgNPs demonstrated particle size of 192-232nm with zeta potential value of +29 to +32.18mV and PDI of 0.28 indicating nanoscale particle formation with good electrostatic stability. A linear ciprofloxacin calibration curve was established with an R^2 value of 0.999. The inclusion of PVA into the formulation allows improving film forming properties and mechanical stability, while flaxseed mucilage can act as a hydrophilic natural biopolymer providing additional moisture retaining capability. The optimized formulation will be prepared via solvent casting technique and evaluated for physicochemical and mechanical properties, including thickness, folding endurance, tensile strength, moisture content, drug content and in-vitro drug release. The structure and morphology will be determined by the methods of Fourier-transform infrared spectroscopy, Xray diffraction and scanning electron microscopy. The antimicrobial effectiveness will be evaluated against selected wound associated microorganism. The developed multi-scaffold film will possess enhanced antimicrobial effectiveness and physico-mechanical characteristics.

Keywords: Silver Nanoparticles, Biopolymer, Solvent Casting Method, Wound Healing

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4.	Ms. Smriti Prasad , Research Scholar, Department of Pharmaceutical Science (MPharm Pharmaceutics), MIT World Peace University, Pune

SPECIAL APPRECIATION AWARD			
S. No	Name	Title of Presentation	Institute
1.	Prof. Dr. Susai Rajendran	The Impact of Specific Chocolate Compositions on the Corrosion Resistance Properties of SS 316 L Alloy when Submerged in Synthetic Saliva	Corrosion Research Centre, St Antony's College of Arts and Sciences for Women (Autonomous), Dindigul & Co-Editor - Materials Protection
2.	Ms. R.J.R Jhoshie Rachal	The Impact of Specific Chocolate Compositions on the Corrosion Resistance Properties of SS 316 L Alloy when Submerged in Synthetic Saliva	Loyola Tech School, Dindigul, Tamil Nadu, India
3.	Ms. Sree Laya	The Impact of Specific Chocolate Compositions on the Corrosion Resistance Properties of SS 316 L Alloy when Submerged in Synthetic Saliva	Loyola Tech School, Dindigul, Tamil Nadu, India

About iNEEBA-2026

The 6th International Conference on Nanoscience and Nanotechnology for Energy, Environment and Biomedical Applications (INEEBA-2026) will be held during September 24-25, 2026. This conference includes keynote lectures from eminent scientists across the world, oral presentation and poster presentation of various aspects of Nanoscience and Nanotechnology. The goal of the conference is to create a platform for materials scientists/physicists/chemists from academic institutions and industries around the world to present breakthroughs in their disciplines favorable to exchange ideas and scientific information. The conference will encompass the latest research advances in nanoscience and nanotechnology with a focus on energy, environment, and biomedical applications. It will highlight innovative approaches for sustainable energy generation and storage, environmental remediation, green technologies, advanced nanomaterials for healthcare, diagnostics, and therapeutics. Thus, the conference on nanomaterials will serve as a multidisciplinary venue for talks and deliberations. The iNEEBA 2026 invites abstracts and full-length manuscripts in the thematic areas of material science and biomaterials for oral/poster presentations and peer-reviewed publications.



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