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ADASPUR, CUTTACK

# Udayanath Autonomous College of Science & Technology

Adaspur, Cuttack – 754011, Odisha, India

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## 8th OCS EXTENDED LECTURE SERIES

## NATIONAL SEMINAR

ON

# FRONTIERS IN CHEMISTRY AND CHEMICAL SCIENCES-2026

**10–11 OCTOBER 2026**

Udayanath Autonomous College of Science & Technology
Adaspur, Cuttack – 754011, Odisha, India




**ORGANIZED BY**

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Udayanath Autonomous College of Science & Technology
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- KEYNOTE TALKS
- POSTER PRESENTATIONS
- EXPERT SESSIONS
- NETWORKING & COLLABORATION

*Exploring Innovations, Advancing Sustainable Future*

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# SOUVENIR 2026

## NATIONAL SEMINAR &
## 8TH OCS EXTENDED LECTURE SERIES

# FRONTIERS IN CHEMISTRY AND CHEMICAL SCIENCES-2026

**FCCS-2026**

**10TH-11TH OCTOBER 2026**


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**"National Seminar and**
**8th OCS Extended Lecture Series 2026"**

***Theme***

**"Frontiers in Chemistry and Chemical Sciences 2026"**

***Organized by***

**Department of Chemistry**
**Udayanath Autonomous College of Science and Technology**
**10-11th October 2026**

| | |
|---|---|
| **VENUE : Gallery, UNC** | |
| **Events** | |
| **Events10th October 2026, Saturday** | |
| **8.30 – 9.30 AM : Registration** | |
| **9.00 – 10.00 AM : Breakfast** | |
| **10.00 -11.00 AM : Inauguration** | |
| **TECHNICAL SESSION-01** | |
| ***Chairperson:*** **Prof. Satyaban Jena, Retd. Professor, Utkal University** | |
| ***Session Coordinator:*** **Dr. Smruti Pattnaik** | |
| **KEYNOTE LECTURE** | |
| **11:00-11:40AM** | **Prof. Ashok Kumar Mishra, IIT Madras**<br>**Topic: "Chemical Science and the Progress of Human Civilization"** |
| **INVITED LECTURES** | |
| **11.40-12.15PM** | **Prof. Pradeepta Kumar Panda, University of Hyderabad**<br>**Topic: "Porphycene – An Emerging 18π Isomeric Porphyrin Dye and its Near Infrared Active 26π-Expanded Analogue"** |
| **TECHNICAL SESSION-02** | |
| ***Chairperson :*** **Prof. Sasadhar Samal, Retd. Principal**<br>***Session Coordinator :*** **Dr. Smruti Pattnaik** | |
| **12:15-12:45AM** | **Prof. Saratkumar Swain, VSSUT, Burla**<br>**Topic:"Chemistry Inspired by Nature: From Natural Phenomena to Advanced Materials"** |
| **12:45-01:15AM** | **Prof. AdinarayanDoddi, IISER Berhampur, Ganjam**<br>**Topic: "N-Heterocyclic Carbenes: Versatile Platforms in Metal-Free and Metal-Based Homogeneous Catalysis"** |
| **LUNCH BREAK : 01.15 TO 02.00 PM** | |
| **POSTER PRESENTATION : 02.00 TO 02.45 PM** | |
| ***Chairperson :*** **Prof. Ashutosh Samantray, Retd. Prof., OUAT, BBSR**<br>**Dr. Asit Parija, Retd. Principal**<br>**Prof. Bigyan Ranjan Das, OUTR**<br>***Session Coordinator :*** **Dr. Shiv Kumari Panda**<br>**Dr. Jay Kishon Swain** | |

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|---|---|
| **TECHNICAL SESSION-03** | |
| **INVITED LECTURES** | |
| ***Chairperson :*** **Prof. Prakash Mohanty, Retd.Prof., Utkal University, BBSR** ***Session Coordinator:*** **Mr. Subrat Nayak** | |
| **2.45-3.15 PM** | **Prof. Himansu Sekhar Biswal, NISER, BBSR. Topic: "IR Spectroscopy of Cosmic Ice and Kidney Stone"** |
| **3.15-3.45 PM** | **Dr. Bikash Jena, Senior Principal Scientist, IMMT, BBSR Topic : "Designing Materials for Multifunctional Energy Storage applications"** |
| **3.45-4.00 PM** | **Prof. Sabita Patel, NIT, Rourkela Topic : "Tailoring Aggregation induced emission (AIE) Fluorophores via Molecular Engineering: From Structural Design to Applications"** |
| **TEAE BREAK (Inside the Hall)** | |
| **TECHNICAL SESSION-04** | |
| **Chairperson : Prof. Ajay Kumar Patnaik, Retd. Prof. Khallikote Autonomous College Session Coordinator: Mr. Guruprasad Dash** | |
| **4.15-4.45 PM** | **Prof. Sabita Nayak, Ravenshaw University, Kataka Topic : "Frontiers in Organic Synthesis: From the Foundations of Classical Chemistry to Artificial Intelligence-Driven Molecular Design"** |
| **4.45-4.55 PM** | **Kabita Mohapatra, J.K.B.K. College, Kataka (Oral)** |
| **4.55-5.05 PM** | **Subhadeep Acharya , Ravenshaw University, Kataka (Oral)** |
| **5.05-5.15 PM** | **Amrita Palai, Kujanga College, Jagatsinghpur (Oral)** |
| **5.15-5.25 PM** | **Mrs. Shriya Bal, Salipur Autonomous College, Kataka (Oral)** |
| **5.30 PM** | **Vote of Thanks with concluding remarks.** |

**"National Seminar and**
**8th OCSExtendedLecture Series 2026"**

***Theme***

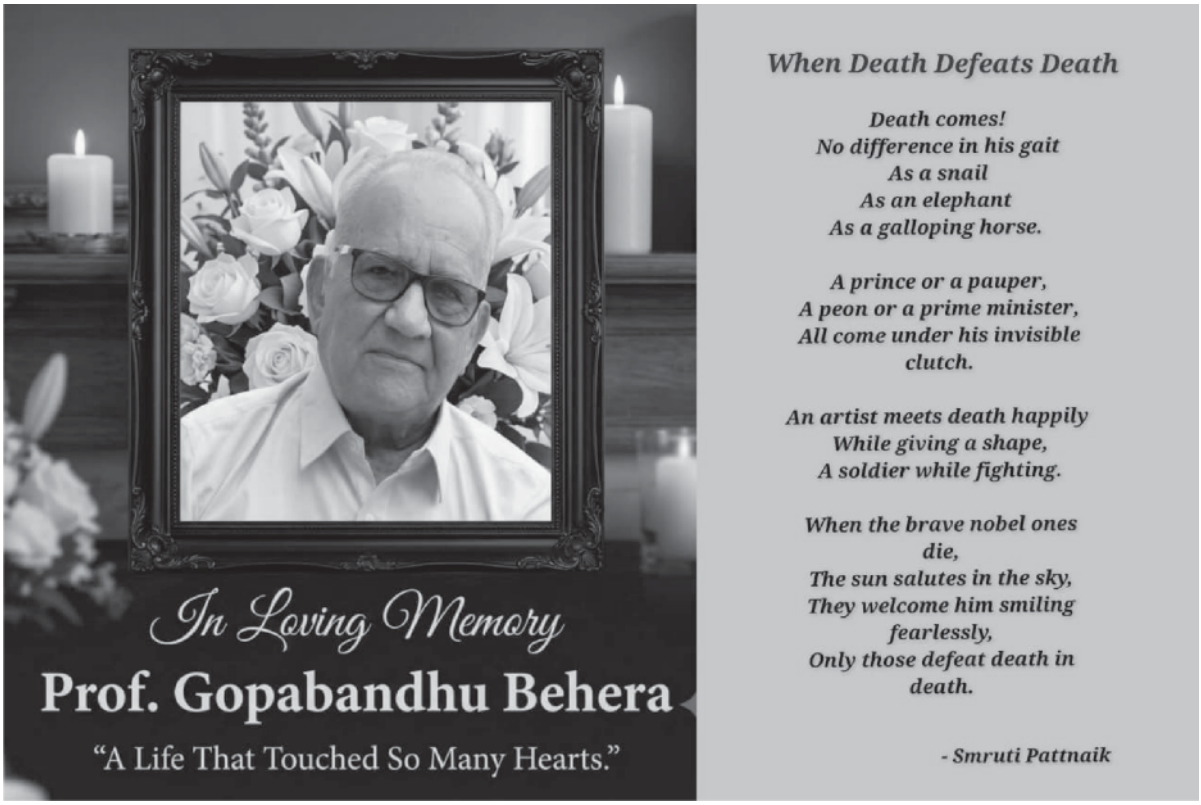
**"Frontiers in Chemistry and Chemical Sciences 2026"**

***Organized by***

**Department of Chemistry**
**Udayanath Autonomous College of Science and Technology**
**10-11th October 2026**

| VENUE : Gallery, UNC | |
|---|---|
| **Time Interval** | **Events** |
| **11th October 2026, Sunday** | |
| **8.30 - 9.30 AM : BREAKFAST** | |
| **TECHNICAL SESSION-05** | |
| ***Chairperson :*** **Prof. Sarata Kumar Das**<br>**Retd. Principal**<br>***Session Coordinator :*** **Dr.Tapaswini Das** | |
| **INVITED LECTURES** | |
| **9.30-10.00 AM** | **Prof.Purnendu Parhi, Ravenshaw University, Kataka**<br>**Topic: "Engineering Rare Earth-Based Heterojunction Composites for Advanced Photocatalytic Degradation of Recalcitrant Organic Pollutants"** |
| **10.00-10.30 AM** | **Prof. Braja Narayan Patra, Utkal University, BBSR**<br>**Topic: "Advanced Polymeric materials for dyes sequestration"** |
| **10.30-11.00 AM** | **Prof. UmaprasanOjha, IIT BBSR, BBSR**<br>**Topic: "Development of Electrodes and Processes for Energy Efficient Green $H_2$ Production from Water"** |
| **TEAE BREAK (Inside the Gallery)** | |
| **TECHNICAL SESSION-06** | |
| ***Chairperson :*** **Prof. Smrutiprava Das**<br>**Retd. Professor, Ravenshaw University**<br>***Session Coordinator :*** **Dr. Tapaswini Das** | |
| **11.00- 11.20 AM** | **Chinmaya Parija, DGM, IFFCO, Paradeep**<br>**Topic: "Chemistry in Fertiliser Industry"** |
| **11.20-11.40 AM** | **Prof. Bibhuti Bhusan Parida, Berhampur University, Ganjam**<br>**Topic: "Green Chemistry for the Sustainable Synthesis of Medicinally Relevant Functionalized Molecules"** |
| **11.40-12.00** | **Dr. Santosh Kumar Behera, Model Degree College, Nayagarh**<br>**Topic: "Impact of Heteroatom Substitution on Photophysis of Dual-State Emissive 2-(2'-hydroxyphenyl)benzazole Dyes"** |
| **12.00-12.10 PM** | **Swadhinswaraj Acharya, Berhampur University, Ganjam (Oral)** |

| | |
|---|---|
| 12.10-12.20 PM | Maksood Alam, IISER Berhampur, Ganjam(Oral) |
| 12.20-12.30 PM | Rageshree Dash, IISER Berhampur, Ganjam (Oral) |
| 12.30-12.40 PM | Aiswarya Moharana, IISER Berhampur, Ganjam (Oral) |
| 12.40- 01.00 PM | Dr. Milan Kumar Jena (Online), IIT Bhilai, Chhattisgarh<br>Topic: "Machine Learning Combined Quantum Transport for High-Throughput DNA Sequencing using Solid-state Nanopore Technology" |
| 01.00-01.15 PM | Dr. Satyaranjan Jena (Online), Taiwan University, China<br>Topic: "Facet and Lattice Engineering of Semiconductor Nanomaterials for Enhanced Photocatalytic and Piezocatalytic Performance" |
| LUNCH BREAK: 1.15 – 2.15 PM | |
| 2.30-4.00 PM | VALEDICTORY WITH CONCLUDING REMARKS |




**03.02.1938 - 22.09.2026**

**On the Eve of**
**8TH OCS EXTENDED LECTURE SERIES**

*Dedicated to*
**LATE PROF. GOPABANDHU BEHERA**
Past President, OCS

# Prof Gopa Bandhu Behera : An Eminent Chemist, Visionary Educationist, Pioneering Researcher and Intellectual Pillar of Odisha

**Prof.Bijay Kumar Mishra**
**Distinguished Professor and Professor of Eminence,**
**Rani Rasomani Green University, Singur,WB**
**President,**
**Indian Society for Surface Science and Technology, Kolkata**
**Ex-UGC BSR Faculty Fellow and Emeritus Fellow,**
**Sambalpur University, JyotiVihar - 78 019**



The global scientific community, and more intimately the fraternity of chemical sciences in India, mourns the deeply saddened passing of Professor (Dr.) Gopa Bandhu Behera, who left this mundane world at 2.40 AM on September 22, 2026, at the age of 87. A pioneering chemist, visionary educationist, and monumental intellectual pillar, Professor Behera passed away at Apollo Hospital, Bhubaneswar leaving behind an irreplaceable void in the fields of physical-organic chemistry, education, and institutional development in Odisha. For over four decades, he served as a beacon of scientific reasoning, inspiring generations of scholars through his prolific research and unyielding commitment to nurturing a logical, evidence-based mindset across society.

His transition marks the end of a golden era in Odisha's higher education system. As a former President of the Orissa Chemical Society, an appellate authority of Odisha Pollution Control Board, a long-serving Professor and Head of the Department of Chemistry at Sambalpur University, and the ideological vanguard behind the educational renaissance of Kalahandi, his legacy remains permanently etched into the structural and intellectual landscape of the State.

Born on February 3, 1939 to Suresh and NirabatiBehera, in the village of Mahichala (Bhursiguda) of Kalahandi district of Odisha, GopaBandhuBehera's journey from a remote rural locality to the apex of academic excellence is a testament to his profound intellect and relentless willpower. After schooling in Manikeshwari High School, Bhawanipatna, he moved to Ravenshaw College in Cuttack to pursue higher studies in science. He completed his B.Sc. (Honours) in Chemistry in 1958, securing the First rank and M.Sc. in Chemistry in second rank in 1960 from UtkalUiniversity.

Professor Behera's research journey began during a transformative phase for Indian chemistry. He pursued his doctoral studies under the guidance of the legendary educator and chemist, Professor Mahendra Kumar Rout. His investigative rigor in heterocyclic dyes systems culminated in the award of a Ph.D. degree from Utkal University in 1969. Recognizing that true science requires deep, persistent exploration, he continued to advance his specialized investigations in Surface Chemistry, which earned him the highly prestigious Doctor of Science (D.Sc.) degree from Sambalpur University in 1978, the first award of Sambalpur University.

His teaching and research career spanned nearly forty years, characterized by a series of foundational academic appointments across prestigious institutions. He began his career as a Lecturer in Chemistry at the Samanta Chandra Sekhar (SCS) College in Puri, serving from 1960 to 1964. He returned to his alma mater, Ravenshaw College, teaching there as a Lecturer from 1964 to 1969. However, his defining institutional legacy was forged at Sambalpur University, where he joined as a Lecturer in 1969, ascended to the position of Reader in 1971, and was appointed Professor of Chemistry in 1978. He held this professorship for a record-breaking 21 years until his retirement in 1999, extending further two years as Emeritus Professor establishing a golden era for the university's School of Chemistry.

As a researcher, Professor Behera was known for his methodological meticulousness. His primary contributions lay at the intersections of physical-organic chemistry, surfactant chemistry, and the kinetics and mechanisms of organic reactions. Over his lifetime, he published more than 120 comprehensive research papers in renowned national and international peer-reviewed scientific journals. He acted as a Guest Editor of Journal of Indian Chemical Society. His work helped unpack complex intermolecular interactions, micellar catalysis, and structural-reactivity relationships in organic substrates. Beyond individual publications, his capability to translate intricate molecular theories into comprehensive lessons meant that he was highly sought after as a research guide, ultimately mentoring sixteen of doctoral and post-doctoral scholars who now occupy prominent scientific chairs across the globe. His research interest is exemplified from his submission of an article in the month of his superannuation to the journal, Chemical Reviews (impact factor 64.2) and the article has received around 2072 citations till date.

Professor Behera's scientific contributions extended far beyond the walls of his laboratory. Believing that science must be organized to grow effectively, he served as a Founder Member and Past President of the Odisha Chemical Society (OCS), Odisha Environment Conscientiousness Society(OECS) and Vice-President of Indian Society for Surface Science and Technology (ISSST). Through the OCS, he initiated various symposia, research workshops, and student outreach programs designed to bridge the gap between regional institutions and global breakthroughs. His efforts earned him deep respect among peer organizations like the Indian Chemical Society, the Indian Science Congress Association and Indian Photobiology Society. In recognition of his lifetime dedication to research and pedagogy, he was explicitly felicitated by the OCS as the first VSR Gupta best teacher award (1995), by the Government of Odisha as a Senior Scientist of the State (2012), celebrating his foundational role in popularizing chemistry and utilizing scientific progress to address societal challenges. He was bestowed upon the Luminary Award by OCS (2024) and Life time contribution award by Indian Society for Surface Science and Technology, Kolkata (2025). In his honour the Prof. G. B. Behera best Ph. D. thesis award has been instituted by OCS to recognize the outstanding doctoral research in Chemical Sciences in the State. The Professor G. B. Behera endowment Lecture, organized annually on his birthday, 3rd February, by the Sambalpur University is an enduring tribute to his contribution to chemistry and education.

## Research Work of Professor GopaBandhuBehera

Working at the intersection of physical chemistry and organic synthesis, his investigations significantly advanced the mechanical understanding of complex molecular interactions. His main scientific endeavors can be synthesized into three core programmatic domains.

### Physical-Organic Chemistry and Reaction Mechanisms

A primary focus of Professor Behera's early and mid-career research was expanding the boundaries of physical-organic chemistry, building on the traditions established during his doctoral work under Professor M. K. Rout. He investigated the kinetics and thermodynamics of a wide variety of organic reactions. His research parsed how changes in molecular geometry, substituents, and environments alter the paths of chemical transformations. By utilizing quantitative linear free-energy relationships (LFER), his laboratory systematically calculated structural-reactivity behaviors in complex organic substrates. This helped chemists predict how structural modifications could influence the velocity and yield of organic syntheses. One of his ground-breaking work includes - derivation of steric density (SD), a substituent parameter to be used in LFER and QSAR.

### Surfactant Chemistry and Micellar Catalysis

Professor Behera was widely acknowledged for his innovative contributions to colloid and surfactant chemistry. As a Fullbright Fellow, he worked in South Florida University, USA (1985) on monolayer of molecules on water surface and extended the work in India to complex microemulsion systems. His laboratory comprehensively explored the physical attributes of micellar systems and how organized molecular assemblies behave in solution. A notable contribution of his team was optimizing micellar catalysis—using self-assembled surfactant aggregates to alter the rates and stereochemical outcomes of chemical reactions. By mapping how the microenvironment of a micelle stabilizes transition states or concentrates reacting molecules, his work provided structural frameworks for modern green chemistry. He proposed different localization sites around micellar systems attributing to hydrophobic force field. This research favored the deployment of aqueous, eco-friendly surfactant mediums to replace hazardous, toxic industrial organic solvents.

### Solvatochromism and Molecular Dyes

His later academic inquiries delved deeply into the study of solvatochromic dyes and their interactions inside varying microheterogeneous environments. Professor Behera investigated how the absorption and emission spectra of specialized organic dyes shift in response to the polarity, viscosity, and local charge of their surrounding solvents. This research acted as a highly precise analytical tool. It allowed scientists to use dyes as molecular probes to chart the structural integrity and internal dynamics of lipid bilayers, microemulsions, polymers, and biological membranes.

Through these interconnected domains, Professor Behera's work bridged the gap between purely theoretical physical equations and practical organic engineering. His quantitative precision not only enriched the fundamental textbook understanding of molecular dynamics but also laid down chemical blueprints utilized today in pharmaceutical formulations, industrial catalysis, and material sciences.

Equally significant was his profile as an institutional builder and social reformer. Professor Behera strongly believed that the ultimate validation of scientific privilege lay in uplifting underprivileged communities through the democratisation of knowledge and he took up the leadership mantle as the President of the Kalahandi ShikshaVikasParishad. He spearheaded a legendary grassroots intellectual movement that advocated passionately for institutional equity. His strategic vision and tireless dialogues with policymakers played a pioneering role in the eventual establishment of vital public institutions in the region, including the Government Medical College, the Government College of Engineering, and the state university structure in Kalahandi. He was also the President of Divine Life Society of Kalahandi district.

To his students, Professor Behera was a saintly, fatherly figure who commanded immense respect across all academic disciplines. He possessed a rare combination of profound erudition and deep human humility. His classrooms were spaces where equations met philosophy, and where students were taught not just how to pass examinations, but how to think independently and live ethically.

Professor Gopa Bndhu Behera's passing marks the conclusion of a monumental chapter in the history of science education in Eastern India. He is survived by a vast network of grieving family members, colleagues, and thousands of students whose lives were fundamentally altered by his mentorship. The most fitting tribute the international scientific community can pay to this great soul is to carry forward his dual mission: to pursue uncompromising research excellence within the laboratory, and to aggressively leverage the light of science to eliminate ignorance and inequality from the wider world.

***



**Dr. Hari Babu Kambhampati**
Governor, Odisha

सत्यमेव जयते

**LOK BHAVAN**
BHUBANESWAR - 751 008

No: 632/2026

5th October 2026

## MESSAGE

I am delighted to know that the Department of Chemistry, Udayanath Autonomous College of Science and Technology, Adaspur, Katak, is organizing the National Seminar and 8th OCS Extended Lecture Series on "Frontiers in Chemistry and Chemical Sciences" on 10th and 11th October 2026. A souvenir is being brought out on this occasion.

Chemistry plays a vital role in addressing some of the most pressing challenges of our times, including sustainable development, healthcare, clean energy, environmental protection and the development of advanced materials. In this context, a seminar focusing on the frontiers of chemical sciences is highly relevant, as it encourages scientific inquiry, interdisciplinary collaboration and the sharing of innovative ideas and research findings.

I am confident that the seminar will provide a valuable platform for scholars, researchers and students to engage with emerging trends and breakthroughs in chemistry, exchange knowledge and perspectives and explore new avenues for research and innovation. Such academic interactions also help inspire young minds to pursue scientific excellence and contribute meaningfully to the advancement of society.

I wish the organizers and participants a highly enriching, fruitful and successful seminar.

**(Hari Babu Kambhampati)**



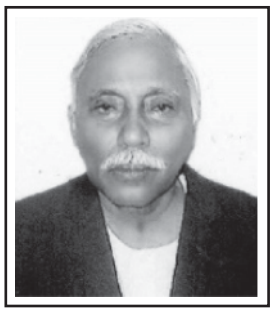
**Prof. Augustee Mohanty**
President
Governing Body, UNC

# Message

I am immensely pleased to learn that Department of Chemistry, Udayanath Autonomous College of Science and Technology, Adaspur, is organizing a National Seminar and OCS Extended Lecture Series on Frontiers in Chemistry/Chemical Sciences-2026. This is a potential platform to encourage interdisciplinary research for our young researchers and academicians. I hope that this academic exercise will help our students and teachers to exchange ideas, present recent scientific advancements and foster collaborations in diverse fields of chemistry and chemical sciences.

The department has time and again achieved accolades for organizing intellectually enriching events. I am sure this will add another feather to its already decorated hat. Wishing this event great success and looking forward to more such constructive endeavour's as future course of action.

**Augustee Mohanty**
**Governing Body President**
**Udayanath Autonomous College of**
**Science and Technology**
**Adaspur, Kataka**



**Sj. Panchanan Kanungo**
EX-Finance Minister, Govt. of Odisha

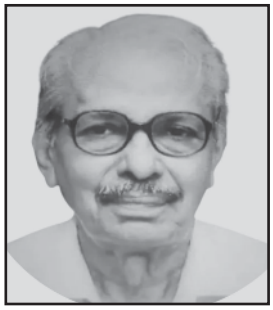
# Message

Public and scientific views on chemistry encompass with fundamental role in understanding the world, its vital industrial and the environmental challenges associated with it. Both organic and inorganic study helps to develop the life of individual and also society is regulated through this study.

I came to know that the chemistry department of U.N. Autonomous college of Science & Technology is organized a seminar in the interest of the students for enhancing their knowledge.

I wish all the success and hope; students are benefited out of this.

With Thanks
**Sj. Panchanan Kanungo**
EX-Finance Minister, Govt. of Odisha
Udayanath Autonomous College of
Science and Technology
Adaspur, Kataka



**Dr. P. B. Tripathy**
Ex-Joint Director, UGC

# Message

I extend my warm wishes for the success of the seminar on Frontier Areas of Research in Chemistry & Chemical Science.

Chemistry, joined with Artificial Intelligence and Quantum Mechanics, can open new paths in targeted drug delivery and synthesis, safe solar-energy storage batteries, nitrogen fixation, biodegradable materials, hydrogen generation from water, and artificial photosynthesis, to name a few.

I hope this seminar opens new vistas for young researchers and inspires them to explore uncharted frontiers.

With best wishes
**Dr. P. B. TRIPATHY**
EX Jt. Director, UGC



**Prof. Nibedita Jena**
EX-Director of Higher Education

# Message

It gives me immense pleasure to convey my warm greetings and best wishes on the occasion of **National seminar and 8th OCS Extended Lecture Series-2026**on the theme of "**Frontiers in Chemistry and Chemical Sciences**."

Chemistry is often described as the central science because it connects physics, biology, medicine, environmental science, agriculture and technology. In the present era, frontiers in chemical sciences are expanding rapidly through green chemistry, nanotechnology, advanced materials, medicinal chemistry, computational chemistry, catalysis, energy storage, and chemical applications of artificial intelligence. Suchacademic forums provide an excellent platform for scientists, teachers, researchers, and students to exchange ideas, present emerging research and develop meaningful academic collaborations.

I extend my sincere congratulations to organisers, distinguished speakers, researchers and participating students and wish the programmea great success and a fruitful exchange of ideas.

I would like to offer my warmest greetings to the organisers, and I wish all the success for the souvenir planned on the occasion.

**Prof. Nibedita Jena**
EX-Director of Higher Education
&
Present Governing Body Member



**Dr. Lulumina Dash**
Principal

# Message

It is a matter of great pleasure for me to know that the Department of Chemistry is organizing the two days National Seminar on "Frontiers in Chemistry and Chemical Sciences-2026.The National Seminar provides a valuable platform for academicians, researchers and students to exchange ideas, share recent development, and deliberate on emerging trends in chemical sciences.

I am particularly happy that our Department of Chemistry has taken this initiative to bring together distinguished experts and young researchers on a common platform.I congratulate the organizing committee, the faculty members and students of the Department of Chemistry for their sincere efforts in making this academic event possible.

I am confident that this seminar will be intellectually stimulating, academically enriching and memorable for all concerned.

I wish the seminar a great success.

**Dr. Lulumina Dash**
**Principal**
Udayanath Autonomous College of
Science and Technology
Adaspur, Kataka



**Dr. Prasant Kumar Dash**
President, OCS

# Message

It gives me immense pleasure to extend my warm greetings and best wishes on the occasion of the **two-day Extended Lecture Series and National Seminar** on the theme **"Frontiers in Chemistry and Chemical Sciences (FCCS)"**, being organized on **10–11 October 2026** at **Udayanath Autonomous College of Science and Technology, Adaspur, Cuttack**.

The purpose of conducting this two-day Extended Lecture Series and National Seminar is to provide a dynamic platform for academic exchange on contemporary research, emerging breakthroughs, and modern applications in the areas of chemical sciences, such as **advanced sustainable materials, green synthesis, nanotechnology, environmental sustainability, and technological innovations**. I am confident that this two-day technical event will provide a brilliant forum for distinguished academicians, research scholars, and bright young students to exchange novel ideas, share recent developments, and foster meaningful scientific collaborations. The insights gained here will undoubtedly catalyze further research and elevate the standards of chemistry across the state of Odisha.

I extend my heartfelt appreciation to the **Governing Body, the Principal of the College, the Head of the Department of Chemistry, and all the members of the Local Organising Committee** of the college for their meticulous planning and dedication in hosting this crucial academic meet. I encourage all delegates, especially our young student members, to actively engage in the technical sessions, share their ideas, and utilize this opportunity to interact with distinguished experts.

I wish the **Extended Lecture Series and National Seminar** a grand success.

Warm regards,

**Dr. Prasant Kumar Dash**
President
Orissa Chemical Society



# REPORT OF THE SECRETARY ORISSA CHEMICAL SOCIETY FOR THE YEAR 2026

**Dr. Anita Pati**
**Secretary, OCS**

Today **8th OCS-Extended Lecture Series of** Orissa Chemical Society is being organized in association with the **National Seminar on "Frontiers in Chemistry/Chemical Sciences-2026** at Department of Chemistry, Udayanath Autonomous College of Science & Technology, Adaspur, Cuttack, Odisha. The theme **Frontiers in Chemistry and Chemical Sciences** represent the rapidly evolving boundaries of chemical research, where fundamental molecular understanding converges with innovation and real-world applications. Therefore the motto of this conference is, Exploring new frontiers, inspiring discoveries, shaping the future through chemistry.

The **Orissa Chemical Society (OCS)**, the apex professional body of chemists in the state, has a distinguished legacy spanning over four decades. Conceived at the School of Chemistry, Sambalpur University, in 1985**,** with **Late Professor Mahendra Kumar Rout** as its Founder President, the Society has grown into a vibrant professional body comprising academicians, researchers, scientists, teachers, and students from India and abroad. With equal emphasis on quality teaching and frontier research in chemical sciences, OCS remains committed to advancing scientific knowledge and fostering academic interaction. Through its **Annual and Regional Conferences, OCS One-Day Extended Lecture Series, OCS–Industry Interface Meets**, and other academic programmes, the Society continues to strengthen chemistry education and research while inspiring young minds towards scientific excellence.

One of the cherished traditions of the OCS is the organization of **Memorial Lectures** during its Annual Conference in honour of eminent chemists whose outstanding contributions have enriched chemical science and inspired generations of students and researchers. Traditionally, five memorial lectures have been organized: the Prof. M. K. Rout Memorial Lecture, Prof. S. R. Mohanty Memorial Lecture, Prof. Gangadhar Sahu Memorial Lecture, CIPET-Sponsored Prof. Padma Lochan Nayak Memorial Lecture, and Prof. Balaram Sahoo Memorial Lecture. This year, the Society has further expanded this distinguished series by instituting two additional lectures, the **Prof. Bhaskar Dash Memorial Lecture** and the **Prof. Gokulananda Mahapatra Memorial Lecture** as a mark of profound respect and tribute to these legendary scientists.

The Orissa Chemical Society also recognizes and encourages excellence among young scientists, research scholars, teachers, and students through a number of prestigious awards. These include the Prof. Dayanidhi Patnaik Memorial Award, Prof. R. C. Tripathy Memorial Award, Prof. G. B. Behera Best Ph.D. Thesis Award, Prof. Manju Misra Award, Prof. Pranabandhu Tripathy Award, Prof. Bimbadhar Nayak Memorial Award, Prof. Dinabandhu Bhatta Memorial Award, and Prof. Donald S. Matteson and Prof. P. K. Jesthi Award, among several others. Through these recognitions, the Society seeks to nurture scientific curiosity, acknowledge excellence, and inspire the younger generation to pursue chemistry with enthusiasm and dedication. The notification inviting applications/nominations for the various awards of the **Orissa Chemical Society**has already been published on the Society's website. Interested and eligible candidates are encouraged to submit their applications in the prescribed format. The **last date for submission of applications is 25 October 2026**.

This year, the **Regional Conference of the Orissa Chemical Society**was held at the **PG Department of Chemistry, Government Autonomous College, Sundargarh**, during **22–23 August 2026**. Two awards hold special significance during the Regional Conference. The **Sarat Chandra Science Promotion Award**recognizes a school teacher for outstanding contributions towards the promotion of science education, scientific awareness, and innovation among school students. At this year's Regional Conference, **Ms. Susmita Joshi, Govt. UGHS Chhatabar, Sundargarh**, was conferred with this prestigious award in recognition of her contributions towards promoting science education among young learners. The **Prof. P. K. Jesthi Award**is presented to the student securing the highest marks in the highest academic programme in Chemistry offered by the institutionhosting the Regional Conference. This year, the award was conferred upon **Miss Gayatri Kandra, M.Sc. Chemistry (2024–26 Batch), Government Autonomous College, Sundargarh**, in recognition of her outstanding academic achievement.

In its continuing effort to nurture scientific aptitude at an early stage, the Orissa Chemical Society organizes the Chemistry Olympiad examination, **OLYCHEM**, for students of Classes XII. Awards and prizes are presented to the top-performing students to encourage them to pursue further achievements in science. For the year 2026, OLYCHEM will be conducted on **1st November 2026** at various centres across Odisha. From this year, the Society is introducing the **OCS–Anuradha M.ScChemistry Competition**to encourage postgraduate students to strengthen their knowledge and engage in scientific and intellectual challenges. The name of the exam has been finalized as, **"OCS-CHEMNET"** and this year the exam will be conducted on **29thNovember, 2026 (Sunday), 10:30 AM –1:30 PM**at various centres across Odisha. Attractive prizes and recognitions have been planned to encourage wider participation of young chemistry students across the state.

The Society will culminate its major academicactivities of the year with the **Annual Conference of the Orissa Chemical Society**, to be organized by the Department of Chemistry, School of Applied Sciences, **KIIT Deemed to be University**, Bhubaneswar, from **19th–21st December 2026**. On behalf of the Orissa Chemical Society, I extend a warm and cordial invitation to all teachers, researchers, scientists, scholars and students to participate actively in these forthcoming academic events and make the event a successful one.

As I conclude this report, on behalf of all the members of the **Orissa Chemical Society**, I express our sincere gratitude to **Prof. Augustee Mohanty, President, Governing Body and Chief Patron,** Udayanath Autonomous College of Science & Technology, Adaspur, for her gracious support and cooperation in hosting the **8th OCS Extended Lecture Series** of the Orissa Chemical Society at this esteemed institution. I also extend my heartfelt thanks to **Dr. Lulumina Dash, Principal and Patron,** Udayanath Autonomous College of Science & Technology, Adaspur, for her wholehearted support, encouragement, and cooperation, which contributed significantly to the successful organization of this academic event.

My sincere appreciation goes to **Dr. Smruti Pattnaik, Convener/Organizing Secretary**, and **Mr. Subrat Nayak, Co-Convener**, for their dedicated efforts and meticulous coordination throughout the programme. I also acknowledge with gratitude the valuable contributions of the entire organizing committee, faculty members, staff, and enthusiastic student volunteers, whose commitment, teamwork, and tireless efforts made this event a success.

May this conference inspire stimulating scientific discussions, meaningful collaborations, innovative ideas**,** and renewed scientific curiosity, particularly among our young participants, encouraging them to explore the emerging frontiers of chemical sciences and contribute to discoveries that shape a better future.

***"Where curiosity meets collaboration, new frontiers of chemistry unfold."***

I wish the 8th OCS-Extended Lecture Series of Orissa Chemical Society and National Seminar on "Frontiers in Chemistry/Chemical Sciences-2026 a grand success. Thank you**.**

Dr. Anita Pati

**Dr. Anita Pati**
Department of Chemistry
School of Applied Sciences,
KIIT Deemed to be University
Bhubaneswar-24, Odisha



# Sharing Feelings from the Core of the Heart: From the Desk of the Chief Editor…

**Dr. Smruti Pattnaik**
Convener/Organizing Secretary

Friends,

A very good morning and a warm welcome to this a two-days"**National Seminar-cum- 8th OCS Extended Lecture series**" topic on "**Frontiers in Chemistry & Chemical Sciences**" on 10-11 October 2026.This event is organized by the Department of Chemistry, in collaboration with the OCS, and under the patronage and guidance of our esteemed college.

I am so delighted that my joy knows no bounds. I know that our budding researchers and pioneers (my students) will drink the experience and memory to the lees. This august occasion will surely be a pathfinder, especially for my students.

I extend my hearty thanks and gratitude to the revered educationist and President of the GB, Mr. AugusteeKanungo, and to our dynamic Principal, Dr. Lulumina Dash, for her unflagging support and cooperation. I also acknowledge the wholehearted support and help of all our sponsors. Every member of the department (both staff and students) deserves appreciation and a pat on the back with a smile.

Last but not least, a big thanks and smiling bouquets go to all the article contributors of the souvenir. I am highly hopeful for a lively, fruitful, and interactive technical session.

Once again, I welcome and thank each and every delegate of this seminar. I am certain that if any minor inconveniences arise, you will bear with them with a benign heart.

Thank you.

With Regards,
**Dr. Smruti Pattnaik**
Convener/Organizing Secretary
HOD, Chemistry

# THEME OF THE SEMINAR FCCS-2026



Chemistry is often described as the central scienceconnecting physics, biology, material science, environmental science,medicine, engineering etc. Rapid developments in chemical research are opening new frontiers and providing innovative approaches to address some of the most important challenges facing the humanity.

The proposed National Seminar on **"Frontiers in Chemistry and Chemical sciences"** and 8th OCS Extended Lecture Series (FCCS-2026) aims to provide a common platform for academicians, researchers, scientists, industrial professionals to discuss recent advances and faster collaborations in diverse fields of chemistry and chemical sciences.

The seminar will focus on the transformation of chemistry from conventional approaches towards sustainable, interdisciplinary, technologically advanced socially relevant research. The seminar seeks to highlight the pivotal role of chemistry in addressing global challenges related to sustainable development, renewable energy, environmental protection, healthcare, advanced materials, nanotechnology in medicines, computational chemistry and industrial chemistry.

A major focus will be on Green Chemistry, Sustainable Chemistry, Nano Materials for Energy and Environmental Solutions, Chemical Dynamics of Pollutants, Innovations for Energy,Environmentand Health which seeks to minimize waste, reduce hazardous substances and develop environmentally responsible chemical processes.

Medicinal chemistry, Chemical Biology and Pharmaceutical Sciences represent another important area of contemporary research. Advance research in artificial intelligence in molecular modelling, green chemistry for plastic and pollutant break down, novel solar-to-fuel energy materials and chemical biology are creating new opportunities at the interface of chemistry and life sciences.

- ★ The seminar aims to provide a platform for sharing recent developments and innovative research in chemical sciences.
- ★ It will promote interdisciplinary collaborations among researchers and academicians.
- ★ It will encourage young researchers and students to explore emerging areas of Chemistry.

By bringing together experts from Academia Research Organizations and Industry, FCCS-2026 aspires to strengthen scientific networking, facilitate technology transfer and contribute to the advancement of Chemical Sciences for the benefit of society and sustainable development.The National Seminar and OCS Extended Lecture Series will therefore provide an opportunity to explore how chemical sciences can contribute to a cleaner environment, better health care, sustainable energy, advanced materials and technological progress.

Ultimately, the National Seminar aims to strengthen the connection between fundamental research, innovation and social needs, while highlighting the vital role of chemistry in building technologically advanced, scientifically empowered future and leading our country towards Vikshit Odisha @ 2036 and Vikshit Bharat @ 2047.

**Mr. Subrat Nayak**
Lecturer in Chemistry,
U.N. A C S T, Adaspur, Cuttack
Co-Convener, FCCS – 2026

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# Chemical Science and the Progress of Human Civilization

**Ashok Kumar Mishra**

**Professor Emeritus, Department of Chemistry, Indian Institute of Technology Madras**

***Email: mishra@iitm.ac.in***

The early human specie "Homo" had started using fire for chemical manipulation of naturally available materials, about 20 lakh years back. There are evidences that by the time the modern human (Homo sapiens) evolved (about 3 lakh years back), they were making use of fire extensively that could induce chemical transformations. The evolution of human civilization is strongly correlated with the evolution of chemical sciences.

Science and Technology have been transforming human civilization at ever accelerating rates, starting from the New Stone Age. In the current era, human civilization has completely transformed in all aspects like communication, transportation, healthcare, economic growth and many other. Significant progress in Science and Technology has enabled significant modification of the ecosystem on Earth that has helped rapid growth of living standard of mankind. However, this has simultaneously created significant challenges to environmental health and the health of a vast range of life-forms. 'Sustainability' has now become a buzz word due to the urgency to create an ecosystem on Earth that will continue to support the life-form on Earth.

This talk will explain how chemistry has played a crucial role so far and will continue to play in future, and why sustainable growth of human civilization will require judicious use chemistry.

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# Porphycene - An Emerging 18π IsomericPorphyrinDye and its Near Infrared Active 26π-Expanded Analogue

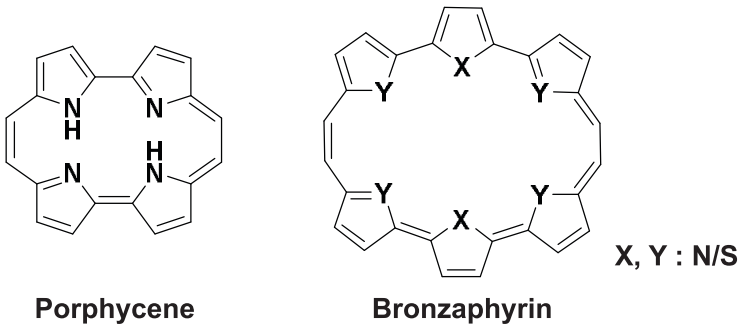
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## ABSTRACT

Porphycene, an 18-aromatic rectangular tetrapyrrole-based macrocyclic dye, is the first constitutional isomer of porphyrin to be reported by Vogel.[1] In spite of its superior ability as a therapeutic in photodynamic therapy compared to the parent isomer, the synthetic difficulties associated with the preparation of bipyrroles limited the development of porphycene chemistry.[2] The presence of two bipyrrolic units make porphycene more responsive towards the effect of substitution. Our efforts towards exploiting this attribute towards tuning the photophysical, structural and coordination chemistry of porphycene unravel several unique features of this macrocycle.[3-4] In addition, some of our efforts towards its near infrared active core expanded 26-hexapyrrolic analogue i.e. bronzaphyrin displaying very interesting structural and functional properties will also be elaborated.[5]




**Porphycene** **Bronzaphyrin**

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# Electron-Transfer Reactions of Biomolecules in the Presence of Keggin-Type 12-Tungstocobaltate(III) in Aqueous Medium.

**Dilip Kumar Baral[1], Guruprasad Dash[2], Prakash Mohanty***

**Christ College, Cuttack**

***PG Department of Chemistry, U.N. Autonomous College, Adaspur, Cuttack, Odisha, India***

## ABSTRACT

The kinetics of electron-transfer reactions of biomolecules, namely **DL-methionine, L-cystine, vitamin $B_6$ (pyridoxine), and NADH**, with **Keggin-type 12-tungstocobaltate(III)** have been studied in aqueous medium. The reactions were investigated over the concentration ranges of **$8.4 \leqslant 10^3$[DL-methionine] $\leqslant 14.0$**, **$1.15 \leqslant 10^3$[L-cystine] $\leqslant 3.5$**, **$0.01 \leqslant$ [pyridoxine] $\leqslant 0.07$**, and **$5.07 \leqslant 10^4$ [NADH] $\leqslant 15.22$ mol dm$^{-3}$**. The corresponding pH ranges investigated for the biomolecular reactions were **3.0–5.0, 2.0–5.0, 3.3–5.0, and 7.0–8.0**, respectively.The products formed in the reactions were identified as **methionine sulfoxide, cystine sulfoxide, 4-pyridoxic acid, and $NAD^+$**, respectively. The activation enthalpy ($\Delta H^{\#}$) and activation entropy ($\Delta S^{\#}$) obtained for the reactions were found to be **$106 \pm 3$ kJ mol$^{-1}$ and $75.75$ J K$^{-1}$ mol$^{-1}$** for DL-methionine; **$16.9 \pm 2$ kJ mol$^{-1}$ and $16.1 \pm 0.5$ J K$^{-1}$ mol$^{-1}$** for the corresponding $K_1$ and $K_2$kinetic pathway; **$-205 \pm 6$ and $-204 \pm 1.5$ J K$^{-1}$ mol$^{-1}$** for $K_1$ and $K_2$ pathway; **$50.84 \pm 6$ kJ mol$^{-1}$ and $-114.2 \pm 14$ J K$^{-1}$ mol$^{-1}$** for vitamin $B_6$; and **$64.14 \pm 2$ kJ mol$^{-1}$ and $-48.9 \pm 6$ J K$^{-1}$ mol$^{-1}$** for NADH.The observed kinetic behaviour indicates that the above electron-transfer reactions proceed predominantly through **outer-sphere electron-transfer (OSET) processes**.

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# Plasma-Assisted Degradation and Mechanistic Investigation of Chlorinated Volatile Organic Compounds

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## ABSTRACT

Increasing environmental concerns and stringent regulations on volatile organic compound(VOC) emissions have encouraged the development of efficient VOC abatement technologies. Non-thermal plasma generated by dielectric barrier discharge (DBD) reactor was employed for the degradation of chlorobenzene, *o*-dichlorobenzene and dichloromethane at atmospheric pressure. The degradation behavior of these chlorinated aromatic and aliphatic VOCs was investigated using different carrier gases (Ar, He, Ar & He along with $O_2$ etc.) to evaluate their influence on plasma-mediated decomposition. The process was performed without an external catalyst and the gaseous products formed during degradation were identified as CO, $CO_2$, and $CH_4$ using GC and GCMS analyses. The by-products deposited on the dielectric surface were characterized by GC, GCMS, FTIR and UV- Vis spectroscopy to determine their chemical structures and stability. Based on the identified products, possible degradation pathways were proposed and evaluated using theoretical gaussian calculations. The results demonstrate the potential of DBD plasma for effective VOC destruction and provide insights for developing plasma-catalyst systems.

**Keywords :** Dielectric barrier discharge (DBD), Non-thermal Plasma, GC(Gas Chromatography), GCMS (Gas Chromatography Mass Spectrometry), Gaussian Analysis.

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# Chemistry Inspired by Nature : From Natural Phenomena to Advanced Materials

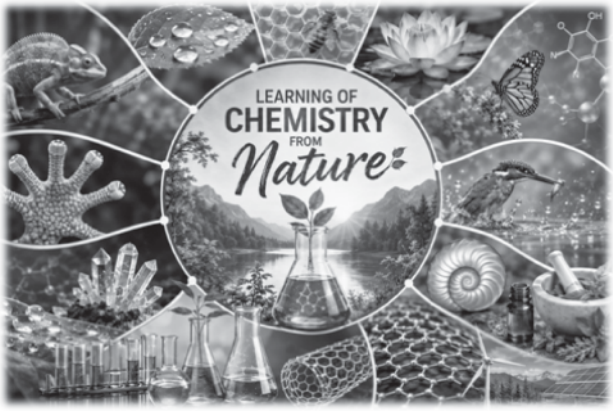
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## ABSTRACT

Nature serves as a fundamental source of inspiration for science and technology. Nature provides a large variety of useful chemical processes and novel materials, such as medicinal plants, natural dyes, colourful flowers, leaves, minerals, and living organisms. The idea of "Learning Chemistry from Nature" points out that the knowledge of natural phenomena may show the fundamental principles of chemistry which can be applied to solve modern scientific problems. Nature has always provided straightforward and efficient mechanisms for generating, arranging, and using molecules and materials in their natural state. Numerous familiar instances in our surroundings can be elucidated using the principles of chemistry and materials science. Plants such as turmeric, neem, tulsi, ginger, aloe vera, and sandalwood contain natural substances with effective and helpful biological qualities. Since the prehistoric ages, natural materials used for medicines, cosmetics, dyes, and fragrances have demonstrated the practical use of chemistry in everyday life. Nature also offers fascinating instances of physical and chemical events. The arrangement of nanocrystals in specialized skin cells is responsible for a chameleon's ability to change colour. Their chemical and physical arrangement alters light reflection, resulting in various colors in response to environmental and physiological factors. The water-repellent behaviour of leaves serves as inspiration for superhydrophobic surfaces and coatings. These features inhibit water adhesion, resulting in high contact angles that allow droplets to roll away and clean surfaces.

Nanomaterials are found naturally in insects, butterfly wings, and bird feathers. Their nanoscale structures regulate light through reflection, scattering, and interference, resulting in dazzling colors without the need of traditional chemical pigments. When sunlight or moonlight interacts with air ice crystals, they produce a halo ring. The refraction, reflection, and dispersion of light through crystal formations results in dazzling circular rings and, in certain cases, colors. When solar charged particles collide with gasses in the atmosphere, the Aurora Borealis is formed. Excited oxygen and nitrogen atoms release energy as coloured light, producing spectacular red, green and violet displays. Likewise, in the presence of oxygen, chemicals such as luciferin and enzymes such as luciferase react chemically to produce bioluminescence. This enzyme-catalyzed mechanism is responsible for the unique colours of marine animals, fungus, and microbes by releasing energy in the form of visible light. The Tyndall effect, halo rings, rainbows and auroras are all examples of occurrences that show how light interacts with matter and how we can explain it with science. Nature is a natural laboratory that keeps shaping chemistry, materials science and technological advancement for us today. The development of nanomaterials and smart materials has also been facilitated by research in nature-inspired chemistry. So, learning chemistry from nature is not about copying nature, it is about understanding the fundamental principles that support natural systems and applying them to design and develop safer, smarter and more sustainable materials.




**Keywords:** Nanomaterials; Nature-inspired chemistry; Sustainable materials; Biomimetic materials; Bioluminescence

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# Designing Materials for Multifunctional Energy Storageapplications

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As a result of the rapid advancement of modern technologies, there is a growing depletion of non-renewable energy sources. This has led to an urgent need forclean, alternative, and extremely efficient energy sources as well as their appropriate storage systems.Modernization in the field of science and technology leads to the advancement of electronic energy storage devices. Nowadays, development in portable electronic devices includes the improvement in performance, reliability, and functionalities of the existing elements as well as the expansion towards flexible miniaturized forms. Supercapacitors are economically sustainable energy storage devices with longer cycle life, rapid charging and discharging time, low internal resistance, and high specific power.They are also capable of operating in extreme temperatures, making them highly versatile. However, despite these advantages, supercapacitors face a significant limitation in their specific energy density, which currently falls short of meeting the energy storage requirements for industrial or practical applications that demand higher energy capacities.To address this challenge, ongoing research focuseson designing materials consisting of both battery type and capacitive materials resulting in higher energy density as well as ultra-high-power density of the energy storage device.

Generally, carbon-based materialshave received extensive research interest as a suitable electrode material for energy storage due to their higher conductivity, greater surface area, high power density, and higher stability.However, several factors like the agglomeration of graphene sheets due to the strong van der Waals forces hinder its vast application. Thus, one of the key goals of the current research is to develop efficient methods for surface engineering carbon-based materials for use in supercapacitors. Similarly, another objective of our work is to produce functional transition metal-based materials, particularly organic-inorganic hybrid structures (metal phosphonates) to increase the high energy density of supercapacitor devices.

**Keywords :** Energy storage, Supercapacitor, Smart devices, Carbon materials, Transition-based materials

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# IR Spectroscopy of Cosmic Ice and Kidney Stone

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**Abstract**

Vibrational spectroscopy is an indispensable experimental technique for probing molecular structures across different physical regimes. While traditional infrared (IR) spectroscopy maps functional group fingerprints, advanced infrared methods ranging from Mid-IR to low-frequency Terahertz (THz) and Vibrational Circular Dichroism (VCD) provide a unified analytical lens for studying molecules and materials. This presentation highlights the versatile application of IR spectroscopy.

In interstellar environments, IR spectroscopy probes low-temperature cosmic ice analogs, unraveling intermolecular hydrogen-bonding networks, lattice motions, and prebiotic chemical evolution under extreme conditions. Conversely, in physiological environments, high-resolution IR methods characterize the molecular architecture, polymorph identification, and crystalline growth mechanisms of pathological biomineralization in kidney stones (nephrolithiasis). By integrating THz low-frequency vibrations and VCD chiroptical signatures, our work at NISER demonstrates how fundamental light-matter interactions elucidate structural symmetry, phase transitions, and molecular composition in both space chemistry and human health.

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# Development of Electrodes and Processes for Energy Efficient Green $H_2$ Production from Water

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## Abstract

The talk will comprise our recent efforts on development of systems and processes for cost effective green $H_2$ production via water electrolysis. Production of $H_2$ via water electrolysis is perceived as the carbon free and environmentally sustainable route to commercialize $H_2$ energy. However, certain drawbacks in terms of energy efficiency, durability and cost of production hinders the above objective. Therefore, a large number of researchers in the domain area are working towards addressing the above obstacles to make the energy form attractive. We have recently developed a number of strategies to improve the synthesize durable electrocatalysts using cost effective transition metals by employing facet engineering those have displayed superior electrocatalytic activity. In this talk, some of our work will be discussed and the key aspects will be highlighted. We have also developed new anode half-cell reactions for use in coupling with HER for energy efficiency H2 production. These results will also be disclosed. A basic understanding of the research work will be displayed for the benefit of undergraduate students.

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# Frontiers in Organic Synthesis: From the Foundations of Classical Chemistry to Artificial Intelligence-Driven Molecular Design

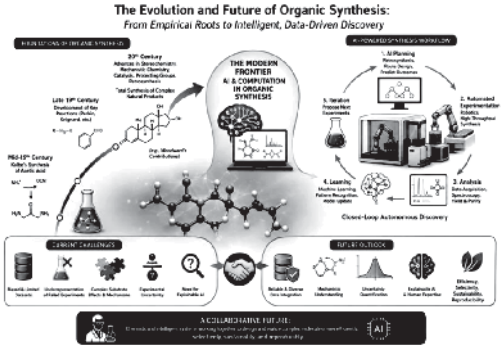
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**Abstract**: Organic synthesis has evolved from an empirical practice into a rational, predictive, and increasingly data-driven science. A major milestone occurred in 1828 when Friedrich Wöhler synthesized urea from inorganic precursors, challenging the doctrine of vitalism and demonstrating that organic compounds could be prepared outside living systems. Hermann Kolbe's synthesis of acetic acid and the subsequent development of reactions such as the Perkin and Grignard reactions further established synthesis as a central discipline of chemistry.[1,2] The contemporary frontier of organic synthesis is being shaped by the integration of artificial intelligence (AI), machine learning (ML), and computational chemistry. Traditional synthesis planning relies strongly on the knowledge and intuition of experienced chemists, whereas AI-based methods can analyze large reaction datasets and identify patterns that may be difficult to recognize manually. Modern ML and deep-learning systems can assist with retrosynthetic analysis, reaction-outcome prediction, reagent and catalyst selection, reaction-condition optimization, and the generation of possible synthetic routes.[3,4] Therefore, future progress will require integration of reliable experimental data, mechanistic understanding, uncertainty quantification, explainable AI, and human expertise. The future of organic synthesis is likely to be a collaborative discipline in which chemists and intelligent computational systems work together to design and experimentally realize increasingly complex molecules, improving efficiency, selectivity, sustainability, and reproducibility.

**Keywords**: Organic synthesis; history of organic chemistry; total synthesis; retrosynthetic analysis; artificial intelligence; machine learning; reaction prediction; computer-aided synthesis planning; autonomous synthesis; chemical discovery




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# Engineering Rare Earth-Based Heterojunction Composites for Advanced Photocatalytic Degradation of Recalcitrant Organic Pollutants

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## Abstract

The increasing persistence of organic pollutants, including synthetic dyes, pharmaceutical residues, pesticides, and industrial effluents, poses a significant threat to aquatic ecosystems and public health. Heterogeneous photocatalysis has emerged as a promising solar-driven Advanced Oxidation Process (AOP); however, the practical application of conventional semiconductor photocatalysts remains limited by rapid electron–hole recombination, narrow visible-light response, and inadequate charge-transfer efficiency. Rare earth-based composite systems have gained considerable attention as an effective strategy for overcoming these limitations. The unique 4f electronic configurations, variable oxidation states, and oxygen-vacancy-inducing characteristics of lanthanide elements enable enhanced light harvesting, improved charge separation, and accelerated interfacial electron transfer. This work highlights recent advances in rare earth-engineered photocatalysts, including cerium, lanthanum, and other lanthanide-modified heterostructures, with emphasis on interface engineering and Z-scheme charge-transfer pathways.

Particular attention is given to a cerium-doped layered double hydroxide (LDH)/graphitic carbon nitride (g-$C_3N_4$) composite, where reversible $Ce^{4+}/Ce^{3+}$ redox cycling and direct Z-scheme architecture promote efficient visible-light-driven degradation of tetracycline and other model organic pollutants while improving catalyst stability and reusability. The discussion also encompasses band-structure modulation, reactive oxygen species generation, degradation mechanisms, and recent developments in scalable photocatalyst design.

Overall, rare earth-based composite systems offer a versatile platform for developing durable, high-performance photocatalysts for sustainable wastewater remediation and environmental protection.

***Keywords :*** *Rare earth composites; Photocatalysis; Z-scheme heterojunction; Cerium; g-$C_3N_4$*

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# Advanced Polymeric materials for dyessequestration

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Dyes are the chemical substance that impart colour to substances. However, due to their non-biodegradable nature and resistance to light and oxidizing agents, they pose a significant threat as persistent water pollutants.Among the diverse array of remediation, the adsorption has garnered global research interest due to its low operational cost, high efficiency, and straightforward synthesis. Recently, Polymeric adsorbents have come to the forefront as advanced materials for removing dyes.Within this class, conducting polymershave emerged as particularly promising candidatesemerge owing to their low cost and excellent reusability.Modification of conducting polymer are essential for increasing the adsorption capacity in manifold. To exponentially enhance their adsorption capacity, structural modifications are essential; these are typically achieved through doping, composite formation, or the introduction of specific functional groups into the polymer backbone. A series of modified conducting polymers are synthesized were synthesized by adopting strategies specifically for dye eradication. The synthesized polymers were characterized by various techniques. The effect of adsorption parameters along with kinetics and thermodynamic parameters are evaluated for the potential application in the real field. These materials exhibit commendable adsorption performance which is suitable for industrial application. Ultimately, this work offers a highly beneficial framework for societal access to clean water.

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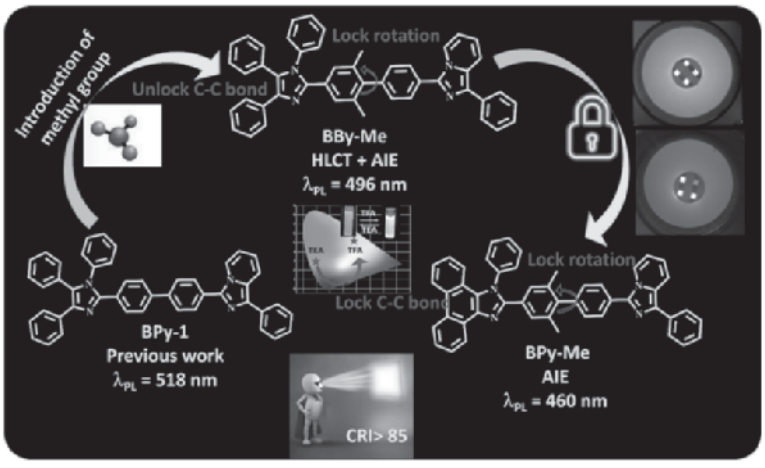
# Tailoring Aggregation induced emission (AIE) Fluorophores via Molecular Engineering : From Structural Design to Applications

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Conventional fluorophores often suffer from aggregation-caused quenching (ACQ) in concentrated states or physiological environments, severely limiting their efficacy in clinical and diagnostic applications. Aggregation-induced emission (AIE) luminogens (AIEgens) overcome this bottleneck by exhibiting enhanced fluorescence upon molecular aggregation, driven by the restriction of intramolecular motions. Consequently, AIE molecules are ideal luminescent material in different solid-state applications especially in OLEDs. Besides OLEDs, AIEgens can be successfully used in chemo-sensing, DNA visualization, fluorescence "turn-on" biosensors, mechano-sensor, protein fibrillation, and specific imaging of cells, organelles, tissues, and microorganisms at molecular, tissue, and cellular levels. In continuation to our endeavour towards exploring several D-π-Abased chromogenic and fluorogenic molecules as solvatochromic, chemosensing and bioimaging probes as well as luminescent materials for OLEDs, we have designed and synthesized different AIEgens by conjugating AIE active moiety to strongly emitting functionalities so as to generate push-pull D-π-AAIEgens. Synthesized luminophores are employed for fabrication of pH sensitive acidochromicmaterials both in solution and solid phase as well as in the generation of white light emitting materials. High-efficiency OLED emitters are fabricated by tuning excited state distributions and by judiciously mixing hybridized local and charge-transfer (HLCT) characteristics with AIE features.




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# N-Heterocyclic Carbenes : Versatile Platforms in Metal-Free and Metal-Based Homogeneous Catalysis

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In recent times, widespread attention has been devoted towards the isolation of main group element consisting species such as silyl phosphines and NHO supported P(III) compounds, these are in fact stereo-electronically tuned phosphorus compounds.[1-3]Stereo-electronically tuned ligands play crucial role not only for the isolation of various novel, and unusual main-group, organometallic fragments, but also find widespread utility as ancillary ligands in homogeneous catalytic transformations. Phosphine ligands featuring group 13/14 elements supported pincer type ligands have been explored [1-3] but their mono-dentate counterparts have not been studied in organometallic synthesis and in homogeneous catalysis. Among this class of species, the silyl (SiR3) groups functionalized phosphines would offer new reactivity aspects as these are sterically, and electronically tuned reactive species. We have recently introduced N-heterocyclic olefin phosphines namely "NHOPs" as potential systems for stabilization of interesting organometallic species and found to be useful in the small molecule (CE2; E = O,S) activation reactions. Carbon dioxide was continently converted to various N-formylated, and cyclic products under metal free conditions. The silylphosphines with Si-H bonds were treated with various Ru and Pd metal precursors and isolated the corresponding Ru(II) and Pd(II) complexes. In the latter case, Pd(II) insertions into the Si-H bonds were observed to give palladium-silicon bonded species, however, the corresponding reactions with R2PSiMe3 afforded P-coordinated complexes, indicating the superior use of Si-H species over Si-R (R = aryl, phenyl) species in organometallic synthesis. 5,6 The details of isolation, structural and catalytic studies will be discussed in this presentation.[4]

**Keywords :** N-heterocyclic olefins, Carbon dioxide, Silver, Phosphine

**References :**

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# Title: Chemistry in Fertiliser Industry, IFFCO, Paradeep

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***IFFCO, Paradeep***

**Abstract**

The presentation provides an overview of the role of chemistry and laboratory analysis in the operation and quality management of the IFFCO Paradeep Fertilizer production. IFFCO Paradeep is a major phosphatic fertilizer manufacturing unit producing Diammonium Phosphate (DAP) and NPK complex fertiliser Ammonium Phosphate Sulphate (NPS).

The unit is supported by itsdifferent sub-units like Sulphuric acid plant, Phosphoric acid plant,Water-treatment Plant, DM Plant, waste Heat Boiler and Power plant and Finished Fertiliser Plant (DAP).

The presentation describes the major chemical processes involved in sulphuric acid, phosphoric acid, and finished fertilizer production, together with the treatment of raw water and production of demineralized water for industrial and boiler applications.

The Central Laboratory of IFFCO is a NABL accredited Laboratory which performs testing of its inhouse samples like Raw Materials, Consumables, Water, Effluents, Emissions, Intermediate, By-products,and Finished Fertilizers.

Laboratory follows systematic procedures involving sample collection, sample preparation, physical and chemical analysis by wet chemicals &instrumental analysisand result reporting.

Apart from basic analytical equipment, the Laboratory is equipped with advanced analytical instruments such as XRF, Atomic Absorption Spectrometer (AAS), Inductively Coupled Plasma Spectrometer (ICPS), UV-Visible spectrophotometers, Segmented Flow Analyser, Automatic nitrogen analysers, ion selective analysers, Bomb calorimeters, and Environmental monitoring samplers.

Overall, the presentation demonstrates how the Analytical Chemistry integrated to Laboratoryanalysisplays one vital roleinFertilizer Production with quality assurance, process control, and environmental compliance at IFFCO Paradeep.

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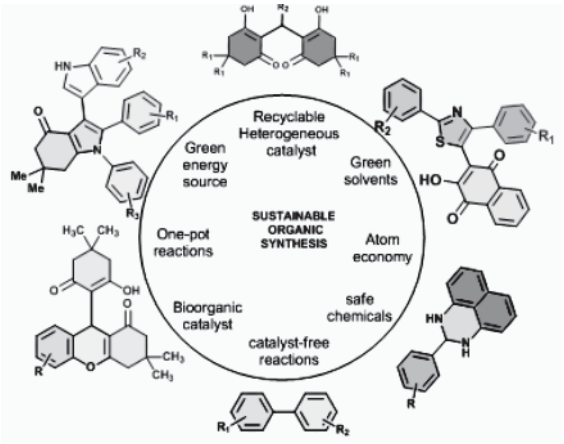
# Green Chemistry for the Sustainable Synthesis of Medicinally Relevant Functionalized Molecules

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**Abstract:**
Sustainable organic synthesis[1,2] is one of the major concerns of chemists for the minimization of waste. In this context, some required approaches are minimizing reaction steps, utilization of green, eco-friendly catalysts, safe, non-toxic substrates, green solvents, avoiding work up steps, and employment of green energy sources. Our group actively works in heterogeneous nanocatalysts, bioorganic catalysis, one-pot multicomponent reactions (MCRs), employment of green energy sources like ultrasonication, and visible light. As part of our on-going research endeavour, we have successfully developed green and sustainable synthetic approaches for medicinally relevant anti-viral tetraketones, dihydroperimidines, fully substituted lawsone-thiazole hybrids,[3] fused functionalized benzopyrans,[4] indole-linked fully substituted fused pyrroles, and also designed recyclable nano Pd-catalysts[5,6] for the synthesis of biaryls by Suzuki-Miyauracross coupling.

**Keywords:** green chemistry, multicomponent reactions (MCRs), functionalized N,O,S-heterocycles, Suzuki coupling, recyclable catalyst




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# Impact of Heteroatom Substitution on Photophysis of Dual-State Emissive 2-(2'-hydroxyphenyl)benzazole Dyes

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**Abstract:**

Organic molecules possessing excited state intramolecular proton transfer (ESIPT) have interesting photophysical properties and have potential application in the field of lasers, UV photostabilizers, sensors, molecular logic gates, light-emitting materials due to their excited state proton transfer ability.[1,2] In this talk, I will be taking about the ESIPT behaviour of , 4-(3-(*1H*-benzo[d]imidazol-2-yl)-5-tert-butyl-4-hydroxybenzyl)-2-(*1H*-benzo[d]imidazol-2-yl)-6-tert-butylphenol (bis-HPBI) and its benzthiazole(bis-HPBT) derivatives. The presence of hetero-atom substitution greatly affects the ESIPT behaviour of these molecules.[3,4]

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# Facet and Lattice Engineering of Semiconductor Nanomaterials for Enhanced Photocatalytic and Piezocatalytic Performance

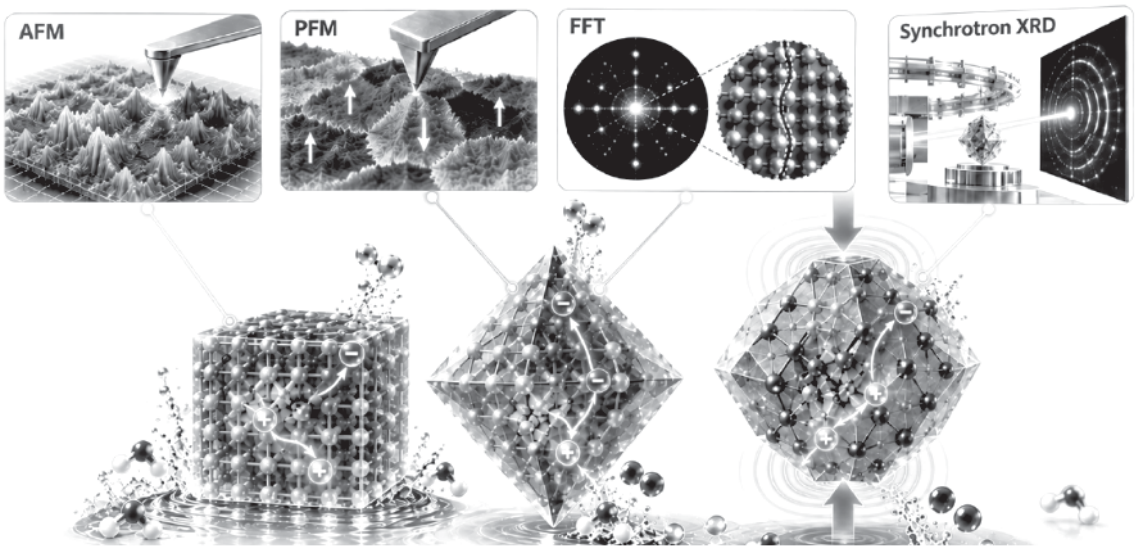
**Dr. Satyaranjan Jena**
**Ph.D. in Chemistry, National Tsing Hua University, Taiwan**

## Abstract

The properties of semiconductor nanomaterials are governed not only by their chemical composition but also by their crystallographic facets, morphology, lattice distortion, and surface structure. Understanding these relationships is essential for designing efficient catalysts and functional materials for energy and environmental applications. This keynote lecture discusses how controlled synthesis and advanced characterization can reveal the connections among crystal structure, charge transport, polarization, and catalytic performance.

The presentation highlights our studies on ZnS quantum dots and nanocubes, ZnSn(OH)6 cubes and octahedra, and related shapecontrolled oxide perovskites. In ZnS nanomaterials, temperature-dependent lattice deviations were correlated with changes in band gap and photoluminescence, demonstrating how subtle structural variations can improve quantum-dot emission.[1] Facet-controlled ZnSn(OH)6 crystals displayed substantial differences in electrical conductivity, piezoelectric response, and dye-degradation performance. The octahedral particles produced a considerably stronger piezoresponse and catalytic activity than the cubic particles, revealing the decisive influence of exposed crystallographic facets.[2] Studies of SrTiO3 and BaZrO3 nanocrystals further showed that morphology, lattice variation, particle size, and exposed facets can regulate optical, photocatalytic, piezocatalytic, and energyharvesting properties. [3,4]

A combination of synchrotron X-ray diffraction, high-resolution transmission electron microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy, UV-visible spectroscopy, photoluminescence, conductive atomic force microscopy, Kelvin probe force microscopy, and piezoresponse force microscopy was employed to establish these structure-property relationships. The lecture also addresses the importance of distinguishing genuine piezocatalytic effects from sonochemical and other mechanically induced contributions. Finally, future opportunities in strain-engineered semiconductor heterointerfaces, piezo-assisted photocatalysis, solar hydrogen production, and operando characterization will be discussed. These findings demonstrate that rational control of facets, lattice structure, and interfacial polarization provides a powerful strategy for developing next-generation nanomaterials for sustainable energy conversion and environmental remediation.




**Keywords :** Facet engineering, Lattice distortion, Semiconductor nanomaterials, Piezocatalysis, Photocatalysis, PFM, and Synchrotron X-ray diffraction.

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# Machine Learning Combined Quantum Transport for High-Throughput DNA Sequencing using Solid-state Nanopore Technology

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**Department of Materials Science and Metallurgical Engineering,**
**Indian Institute of Technology Bhilai, Durg, Chhattisgarh 491002, India**
**Email: milanjena@iitbhilai.ac.in**

**Abstract**

Solid-state nanopore sequencing based on quantum tunnelling offers a promising approach for rapid, label-free, single-molecule DNA sequencing.However, the strong dependence of quantum transport signals on nucleotide orientation and configuration makes obtaining reliable electronic signatures computationally demanding. In this work, we combine machine learning (ML) with quantum transport calculations to develop an artificially intelligent nanopore for high-throughput DNA sequencing.Using 2D solid-state nanopores, quantum transport calculations are performed for different nucleotides at differentdynamic orientations to generate characteristic transmission signatures.These data are used to train ML models to learn the complex relationship between electrode-nucleotide configuration and quantum transport response.The trained models can predict transmission signatures for previously unseen configurations and distinguish nucleotides from their quantum transport fingerprints. This ML–quantum transport framework significantly reduces the need for computationally intensive calculations and provides a promising pathway toward rapid, high-throughput, and high-precision single-molecule DNA sequencing.

1. Jena, M. K.; Pathak, B. Development of an Artificially Intelligent Nanopore for High-Throughput DNA Sequencing with a Machine-Learning-Aided Quantum-Tunneling Approach. *Nano Lett.* 2023, 23 (7), 2511-2521.
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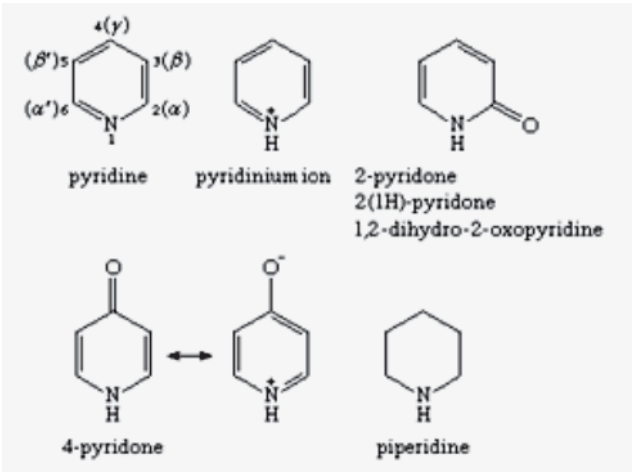
# SIX MEMBERED HETEROCYCLIC COMPOUNDS

**Dr. Smruti Pattnaik**
**HOD, Dept. Of Chemistry**
**U. N. Autonomous College,Adaspur**

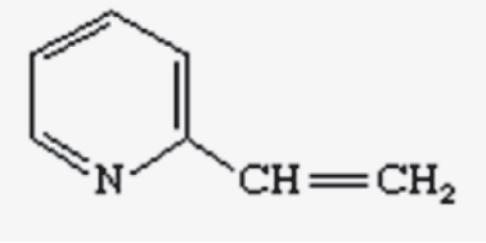
Heterocycles are one of the largest classes of organic compounds worldwide. They are formed through a process known as heterocyclic synthesis, where carbon atoms and at least one heteroatom – non-carbon atom – bind into a ring.

**Six-membered rings with one heteroatom**

The nomenclature used for the various monocyclic nitrogen-containing six-membered ring compounds is given below. Positions on the ring are shown for pyridine, Arabic numerals being preferred to Greek letters, although both systems are used. The pyridones are aromatic compounds because of contributions to the resonance hybrid from charged resonance forms such as that shown for 4-pyridone.



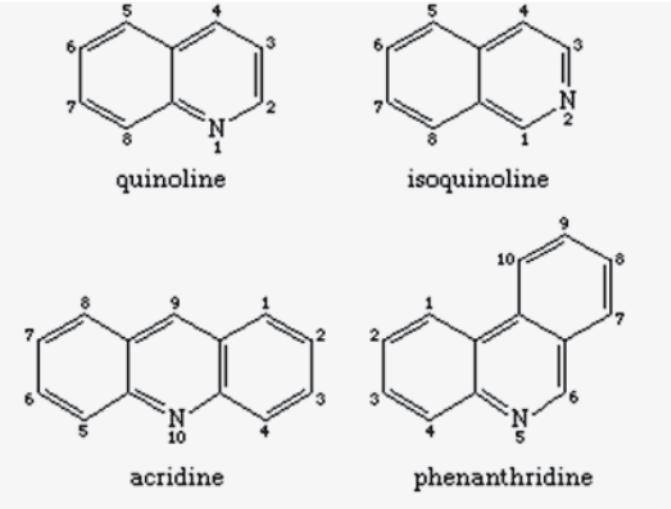

Pyridine, which once was extracted commercially from coal tar but now is prepared catalytically from tetrahydrofurfuryl alcohol and ammonia, is an important solvent and intermediate used to make other compounds. Vinylpyridines such as



are important monomer building blocks for plastics, and fully saturated pyridine, piperidine, is used in rubber processing and as a chemical raw material.

Pharmaceutically important pyridines include the tuberculostat isoniazid (isonicotinic acid hydrazide), the anti-AIDS-virus drug nevirapine, the vasodilator nicorandil, used for treating angina, the urinary-tract analgesic phenazopyridine, and the anti-inflammatory sulfa drug. 1-(1-phenylcyclohexyl) piperidine (PCP, phencyclidine) was originally used as an anesthetic, but its powerful hallucinogenic properties have led to abuse. Diquat, paraquat, clopyralid, and diflufenican are well-known pyridine derivatives used as herbicides.

`Shown in the structural formulas below are two isomeric benzopyridines (upper pair) and two isomeric dibenzopyridines (lower pair), with their common names and accepted numberings. All four compounds and some of their alkyl derivatives have been obtained from coal tar. Each of them is also the parent substance of a class of alkaloids. Of these, the quinolines (e.g., quinine and other derivatives, still obtained from the Cinchona tree) and the isoquinoline (e.g., morphine) groups are particularly well-known.




**KEY WORDS :** Heterocycles , Pyridine.

**REFERENCES :**


- https://www.britannica.com/science/heterocyclic-compound/Six-membered-rings-with-one-heteroatom
- https://pubs.acs.org/doi/10.1021/acs.joc.7b00758


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# Importance of Organometallic Compounds in Chemical Sciences

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**Abstract:**

Organometallic chemistry is an important branch of chemical science that deals with compounds containing metal carbon bonds. These compounds possess unique structural, electronic, and chemical properties, making them valuable in various areas of Chemistry. This abstract highlights the fundamental features and importance of organometallic compounds, particularly their role in catalysis, organic synthesis, polymerization, pharmaceuticals, and material sciences. Their ability to facilitate chemical transformations with high efficiency and selectivity has made them important in both academic research and industrial processes. Organometallic compounds also provide useful insights into metal-ligand bonding, reaction mechanism, and development of new catalytic systems. Important applications such as cross- coupling reactions and polymerization demonstrate their practical significance in modern chemical synthesis. Thus, the study of organometallic chemistry contributes significantly to the development of efficient synthetic method and advanced chemical technologies.

**Key words :**
Organometallic chemistry,catalysis, organic synthesis,chemical technologies.

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# Bio-based hydrogels as multifunctional platforms: recent advances and future perspectives.

**Durgaprasad Mishra**

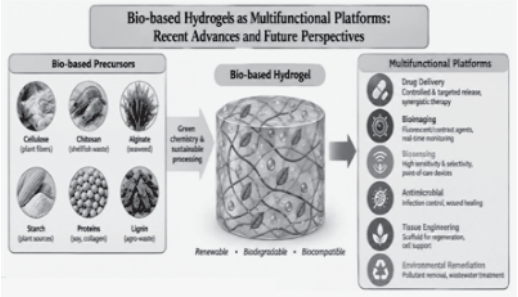
*Udayanath Autonomous college of science and Technology, Adaspur, Kataka.*

**Abstract :**

Hydrogels derived from renewable biopolymers such as cellulose, chitosan, alginate, gelatin, silk fibroin and hyaluronic acid have emerged as versatile soft-matter platforms at the interface of materials chemistry, biomedicine and environmental engineering. Their intrinsic biocompatibility,biodegradability,hydrophilicity and extracellular-matrix-mimetic architecture make them attractive alternatives to petroleum-derived synthetic networks. Recent progress in dynamic covalent chemistry, supramolecular assembly, double-network design and nanofiller integration has enabled precise control over mechanical strength, swelling behaviour, degradation kinetics and stimuli responsiveness (pH, temperature, light, redox, enzymatic). Incorporating functional nanomaterials, including metal and metal-oxide nanoparticles, nanocellulose and carbon-based nanodots, has further imparted antimicrobial, antioxidant, photoluminescent and conductive functionalities. As a result, bio-based hydrogels now serve as wound dressings, controlled drug and gene delivery vehicles, tissue-engineering scaffolds, bioinks for 3D printing, biosensors, and adsorbent matrices for water remediation. This review critically summarizes recent developments in polymer sourcing, crosslinking strategies and structure-property-function relationships, and discusses how these design principles translate into application-specific performance. Persistent challenges are also examined: batch-to-batch variability of natural polymers, limited mechanical robustness under physiological load, long-term toxicological assessment, sterilization, regulatory approval and scalable green manufacturing. Finally, emerging directions are outlined, including machine-learning-guided formulation, 4D bioprinting, closed-loop theranostic hydrogels and circular-economy-oriented production, to guide the rational development of next-generation, clinically and industrially translatable systems.

**Keywords:** bio-based hydrogels; biopolymers; stimuli-responsive materials; nanocomposite hydrogels; wound healing; drug delivery; sustainable materials.

**Graphical Abstract:**




***

# Comparative Surface Characterization of Orthopedic Implant Materials

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**Adaspur, Katak**

**Abstract**

Surface properties of orthopedic implant materials critically govern protein adsorption, cellular interactions, corrosion resistance, and subsequent implant–tissue integration. This study systematically compared the surface morphology, chemical composition, and topographical characteristics of clinically relevant materials used in orthopedic surgery and traumatology. The investigated specimens comprised anodized commercially pure Grade 2 titanium (Ti2), Ti6Al4V alloy with titanium plasma-sprayed (TPS) coating, stainless steel (SS), CoCrMo alloy (CoCr), highly cross-linked ultrahigh molecular weight polyethylene (HXL-UHMWPE), and conventional ultrahigh molecular weight polyethylene (UHMWPE). Surface morphology and elemental composition were characterized by scanning electron microscopy coupled with energy-dispersive spectroscopy (SEM–EDS), whereas surface chemical states were evaluated using X-ray photoelectron spectroscopy (XPS). Surface topography and roughness were quantified by atomic force microscopy (AFM) and profilometry. Among the investigated materials, TPS-coated titanium exhibited markedly greater surface roughness (Ra = 25 ± 2 μm), followed by CoCr (535 ± 19 nm), Ti2 (227 ± 15 nm), and SS (170 ± 11 nm). HXL-UHMWPE and UHMWPE displayed comparable roughness values of 147 ± 13 and 144 ± 15 nm, respectively. EDS confirmed the characteristic elemental constituents of each material, while XPS provided complementary information on their surface chemical states and revealed a substantial contribution of Ti4+ species on Ti2 and TPS surfaces, consistent with titanium oxide-rich surface layers. Collectively, the results demonstrate pronounced material-dependent differences in surface architecture and chemistry. Such comprehensive physicochemical characterization provides an essential basis for correlating implant surface properties with biological responses and for rational optimization of orthopedic implant surfaces to enhance biointegration, functional stability, and long-term clinical performance.

**Keyword:** Orthopedic Implant, Surface Characterization, Chemical composition, Surface Morphology, Roughness

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# Synthesis of Cellulose-Grafted-Chitosan Based Novel Green Superabsorbent for Personal Health care Application

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**U.N Autonomous College of Science & Technology, Adaspur, Cuttack**

**Abstract :**

Chitosan is a polysaccharide based nontoxic green polymer having poly-cationic tendency with inbuilt antibacterial and antifungal qualities. It is biocompatible with various organic and inorganic complexes due to its free -NH 2 and –OH functionalities. These existing groups can easily connect with other functionalities through electrostatic forces of attraction or intermolecular H-bonding. Also, cationic nature of chitosan makes it able to fix with negatively charged end of bacterial cell membranes. Chitosan has the characteristics of solubility in dilute acid solutions and can be fixed with polyanions to form complexes and gels. So specifically the presence of -NH 2 and -OH groups, chitosan can prove it as a potential candidate to transfer it to various interesting forms. Chitosan can be effectively attached with natural polymer like cellulose via crosslinking and grafting techniques, as both have chemical and physical structural similarity. Therefore, this work plan expects the miscibility of chitosan and cellulose. This chitosan can introduce the amino group into cellulose by replacing the inherent -OH group present in the cellulose backbone. Here for both the natural polymers, N-methylmorpholineoxide is used as the suitable polar solvent material which has autocatalytic degradation tendency due to the formation of N-(methylene) morpholinium ion. Here the uniqueness of the work is based on the application of microwave irradiation over the standard thermal treatment to carry out the synthesis of our desired product. Such unique method can offer the properties like uniformity, least energy utility, maximum efficiency, time saving and atom economy. Microwave assisted synthesis mechanism works faster and better than the traditional heating method. Simply it is based on the twelve principles of Green chemistry& that can increase the kinetics of the polymerization process quickly and enhance the whole characteristics of the products in our desired way.

**Key words:** Chitosan, polysaccharide, green polymer, Microwave assisted Synthesis, poly-cationic tendency.

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# Peroxymonosulfate-Assisted Photo-Fenton Degradation of Tetracycline Hydrochloride Using $Fe_2O_3$/B-Doped g-$C_3N_4$) Photocatalysts: Kinetics, Parameters, and Mechanism

**Guruprasad Dash, Kundan Kumar Das, Arjun Behera, Kulamani Parida**
[1] **Department of Chemistry**
**UdayanathAutonomous College of science and Technology, Adaspur**
**Centre for Nanoscience and Nanotechnology, SOA (Deemed to be University), Bhubaneswar-751030, Odisha (India)**
**PG Department of Chemistry, N.C. Autonomous College, Jajpur-755001, Odisha**

## Abstract

Growing environmental degradation, energy scarcity, and the need for proficient intellect from various research groups are the foremost issues in recent times, largely due to the unanticipated surge in capitalism and human activity. Hence, to eradicate such limitations, unchangeable and durable alternatives based on renewable resources are a key challenge for the entire scientific community. This study details the synthesis $Fe_2O_3$-modified boron-doped graphitic carbon nitride (B-doped g-$C_3N_4$) or (BCN) nanocomposites (FeB) for the photocatalytic degradation of tetracycline (TC). The composites were prepared with varying $Fe_2O_3$ loadings (2.5, 5, and 7.5 wt%, labeled 2.5-FeB, 5-FeB, and 7.5-FeB) and characterized using XRD, SEM, TEM, XPS, and UV–Vis DRS. The 5-FeB sample demonstrated the highest performance in a peroxymonosulfate (PMS)-assisted photo-Fenton process under visible light. This enhanced activity stems from a synergistic interaction between $Fe_2O_3$and BCN that improves charge separation, accelerates Fe(II)/Fe(III) redox cycling, and boosts reactive oxygen species (ROS) generation. Consequently, the 5-FeB nanocomposite is a highly promising material for removing pharmaceutical pollutants from wastewater.

**Keywords:** Photocatalysis, PMS-assisted photo-Fenton, tetracycline and nanomaterials.

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# Catalyst and Base Free Aza-Michael Addition Reaction: Synthesis of Poly-substituted 4-Pyrazole Based Benzopyrans

**Tapaswini Das, Seetaram Mohapatra**
*Ravenshaw University, Cuttack*

**Abstract :**

Densely functionalized 2, 3, 4-trisubstituted chromane derivatives and their 4-amino skeletons are the most important structural building blocks of many bioactive natural and unnatural alkaloids possessing potent biological activities such as bactericides, antioxidant, anti-hypertensive, anti-cancer agents and in medicinally enriched drug candidates such as cromakalim, NIP-142, etc [1]. Amongst the procedures available in chemist's toolbox for the construction of 2, 3, 4-trisubstituted aminochromane, aza-Michael addition reaction has emerged as a very popular method and also plays major role in providing ubiquitous nitrogen-oriented essential skeletons in modern organic synthesis [2]. On the other hand, pyrazole is a synthetically interesting heterocyclic molecule shows fascinating therapeutic activities [3]. Considering the biological abundances in many potent drug candidates of 2,3,4-trisubstiuted aminochromanes & pyrazole, herein, an efficient and catalyst free protocol has been disclosed for aza-Michael addition reaction of pyrazoles with 2-aryl-3-nitro-2*H*-chromene derivatives, which provides synthetically important 4-pyrazole-3- nitrobenzopyrans **3(a-s)** at room temperature. The starting material 3-nitro-2*H*-chromenes **1(a-m)** were synthesized by *oxa*-Michael-aldol condensation reaction of substituted salicylaldehydes and trans-*β*- nitrostyrene derivatives in the presence of DABCO as base in toluene at 80 oC. In this one-pot transformation, good to excellent yield of the products up to 84% were obtained and generated a new C-N bond. The relative configuration of the product was characterized by a single crystal X-ray crystallography. Wide substrate scope, high yields, cost-effective, easy accessible, as well as base and catalyst free condition are the major features of the protocol. Moreover, the synthesized Michael adducts **3** were further undergoes amination reaction to provide 4-amino-3-nitro benzopyrans.

**Keywords:** Aza-Michael addition, 3-nitro-2*H*-chromenes, pyrazole, Single crystal X-ray, 2, 3, 4-trisubstituted amino chromane.

**Acknowledgement:** I wish to express my sincere gratitude to Dr. Seetaram Mohapatra for his valuable guidance & support throughout my research work. I am thankful to the H.O.D of Department of Chemistry, U.N. autonomous college of science and tech. for giving me such opportunity.

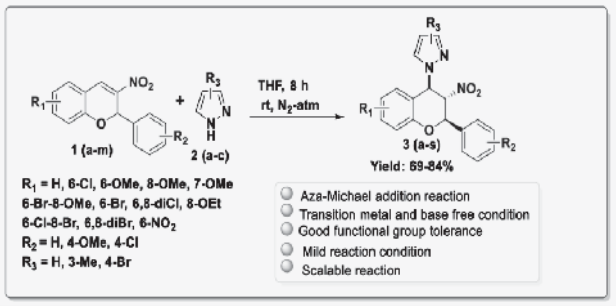



**Fig. 1** *Synthesis of 2,3,4-trisubstituted amino-2H-chromane.*

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3. M. Faisal, A. Saeed, S. Hussain, P. Dar, F. A. Larik, *J. Chem. Sci.* 131 (2019)70.

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# Spent Catalyst-Derived Mo-MOF: Triboelectric Nanogenerators and Energy Harvesting

**Dr. Jaykishon Swain & Dr. Rojalin Sahu**

*U N Autonomous College of Science and Technology, Adaspur, Cuttack*

*KIIT, Deem University, Bhubaneswar-751024, India*

**Abstract:**

Spent catalysts generated during chemical manufacturing are a significant source of environmental pollution and are classified as hazardous waste. However, adopting sustainable waste management strategies such as recycling, recovery, and reuse allows these spent catalysts to be chemically processed for the extraction of valuable metals and salts. This approach not only mitigates waste disposal challenges but also supports the development of a circular economy. In the present study, $MoO_3$ is extracted from a spent petroleum catalyst (Mo–Ni/$Al_2O_3$) and subsequently utilized for the synthesis of a molybdenum-based metal–organic framework (Mo-MOF), with imidazole serving as the organic linker. The structural, morphological, and thermal properties of the synthesized Mo-MOF are systematically investigated. The prepared Mo-MOF exhibits enhanced surface roughness and a positive surface potential. A Mo-MOF/Kapton-based triboelectric nanogenerator (TENG) is fabricated which generates an output voltage of 148 V, a current of 470 nA, and a charge of 17 nC. The TENG is further employed to charge capacitors and power electronic devices, highlighting its practical applicability. Additionally, repetitive boxing punches and exercise motions are successfully monitored using the TENG, indicating its potential for intelligent sports monitoring and healthcare applications.

**Keywords:** TENG, Mo-MOF, 3Rs, Waste to wealth, Sports Monitoring, Healthcare

***

# ZERO WASTE LIFE STYLE FOR A SUSTAINABLE FUTURE

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**Retired Reader in Chemistry**
**Gopabandhu Science College, Athagarh**

## ABSTRACT

**The urgent demand for a greener planet requires sustainable practices. This paper highlights a practical journey towards a zero-waste lifestyle, demonstrating how chemical principles guide waste reduction, reuse, and transformation at the household level.**

**The objective of this work is to reduce household waste through systematic segregation, composting, and innovative reuse of non-recyclables, thereby preventing their accumulation in landfills and reducing environmental pollution.**

**The major findings are with chemical awareness of materials such as biodegradability, polymer properties, combustion behaviour, and toxicity, up to 85% of household waste can be prevented from reaching landfill. Reuse projects, such as converting plastics into mats, bags, pouches, and other household articles, delay polymer degradation and leaching of harmful additives into the environment.**

**The major implications of this study are that sustainable solutions to waste management require not only social commitment but also application of chemical principle at the grassroots level. Systematic waste management will have a positive impact on the general health and hygiene of the society. Particularly it will take care of the dignity and safety of the waste handler. Moreover, integrating waste-to-resource chemistry projects into educational institutions can inculcate scientific awareness among students, building environmentally conscious citizens for the future.**

**Key words***: Conscious citizens, Sustainable practices, zero waste life style, Segregation,Composting,Reuse projects, Community work.*

***

# Influence of Ethylene Glycol and Dimethylformamide Precursor Solvents on the Properties of Selenium-Annealed $Sb_2(S,Se)_3$ Thin Films

**Shriya Sakul Bal , Dibakar Behera and Udai P. Singh**

***School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT), Deemed to Be University, Bhubaneswar - 751024, IndiaSchool of Electronics Engineering, Kalinga Institute of Industrial Technology (KIIT), Deemed to Be University, Bhubaneswar - 751024,India***

## Abstract

Antimony sulfo-selenide ($Sb_2(S,Se)_3$) thin films were prepared using chemical spray pyrolysis with ethylene glycol (EG) and dimethylformamide (DMF) as precursor solvents, followed by selenium annealing at 350°C and 450°C. The influence of solvent type and annealing temperature on the structural, compositional, and optical properties of the films was systematically investigated. X-ray diffraction analysis confirmed the successful formation of polycrystalline $Sb_2(S,Se)_3$ thin film with good phase purity after selenium incorporation. The crystallite size was found to vary between 19.59 and 22.11 nm, with DMF-derived films exhibiting larger crystallite sizes, lower microstrain, and lower dislocation density compared to EG-derived films. Williamson–Hall analysis further supported the improvement in crystallinity and revealed low lattice strain in all samples. EDX-RF measurements confirmed selenium incorporation into the initially deposited $Sb_2S_3$ films and indicated compositional variations with annealing temperature. Optical characterization using UV–Vis spectroscopy revealed direct optical band-gap values in the range of 1.18–1.22 eV. A slight reduction in band gap was observed with increasing annealing temperature, attributed to enhanced selenium incorporation and improved crystal growth. Urbach energy analysis indicated the presence of localized states associated with structural disorder and defect-related band-tail states. Among all investigated samples, the DMF-derived film annealed at 450°C exhibited the best overall structural and optical characteristics, including the largest crystallite size and lowest band-gap energy. The results demonstrate that both solvent selection and annealing temperature play significant roles in tailoring the properties of $Sb_2(S,Se)_3$ thin films, highlighting their potential for photovoltaic absorber layer applications.

***Keywords :*** *$Sb_2(S,Se)_3$ thin films; Selenization; Chemical spray pyrolysis; Williamson–Hall analysis; Optical band gap; Photovoltaic absorber*

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# Catalytic Transfer Hydrogenation of Lignocellulosic Biomass Model Compounds Furfural and Vanillin with Ethanol by an Air-Stable Iron(II) Complex

**Rahul Ghosh, Rakesh R. Behera, Surajit Panda, Sandeep K. Behera, Narayan Ch. Jana, and Bidraha Bagh**

***School of Chemical Sciences, National Institute of Science Education and Research (NISER), An OCC of Homi Bhabha National Institute, Bhubaneswar, PO Bhimpur-Padanpur, Via Jatni, District Khurda, Odisha, PIN 752050, India***

The valorization of lignocellulosic biomass into value-added chemicals requires sustainable and selective catalytic methods. Herein, an air-stable iron(II) complex supported by a tridentate NNO pincer ligand was synthesized from a readily available iron precursor and investigated for catalytic transfer hydrogenation of the biomass-derived aldehydes furfural and vanillin. Using ethanol as an environmentally benign hydrogen donor and solvent, the catalyst selectively converted furfural to furfuryl alcohol and vanillin to vanillyl alcohol in the presence of catalytic KOtBu. Under the most favored conditions for vanillin (2 mol% catalyst, 5 mol% KOtBu, ethanol, room temperature, 8 h), quantitative conversion and excellent isolated yield were achieved. Isopropanol was also effective as a hydrogen donor, generally providing faster conversions. The catalytic protocol tolerated a range of structurally related aldehydes and biomass model compounds, showing high chemoselectivity for aldehyde reduction even in the presence of cyano, nitro, ester, and C=C functionalities. Stoichiometric and kinetic studies supported a catalytic cycle involving iron(II)-alkoxide and iron(II)-hydride intermediates, with β-hydride elimination proposed as the rate-determining step. Gram-scale reactions demonstrated the robustness of the system. CHEM21 green metrics further indicated favorable sustainability characteristics, particularly for the room-temperature ethanol protocol. The study therefore demonstrates an earth-abundant iron catalyst for sustainable transfer hydrogenation of biomass-derived aldehydes using alcohols as hydrogen sources.

**Keywords:** *biomass valorization; transfer hydrogenation; iron catalyst; vanillyl alcohol; furfuryl alcohol*

***

# Transition metal- and base-free [3+2] Cycloaddition mediated synthesis of Isoxazolidines Derivatives and Antibacterial evaluation with Molecular Docking Investigation as DNA gyrase inhibitors

**Kabita Behera1, Suhasini Mohapatra1, Sabita Nayak1*, Seetaram Mohapatra1, Chita Ranjan Sahoo**

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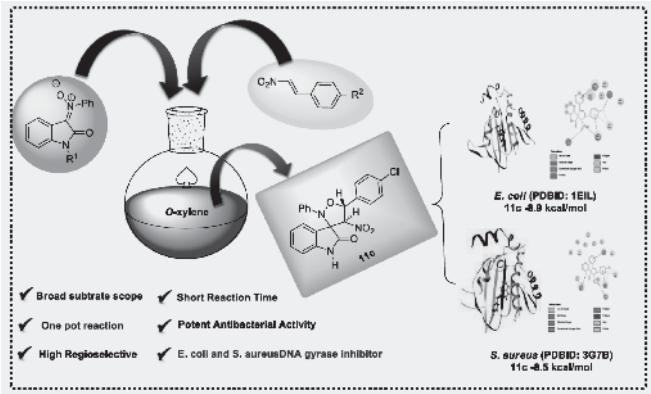
*ICMR-Regional Medical Research Centre, Department of Health Research, Ministry of Health & Family Welfare, Govt. of India, Bhubaneswar-751023, Odisha, India*

**Corresponding author : Dr.Sabita Nayak,** Department of Chemistry, Ravenshaw University, Cuttack-753003, Odisha, India, Email: sabitanayak18@gmail.com

**Abstract:**

A convenient and applicable approach for constructing diverse functionalized 4'-nitro-2',5'- diphenylspiro[indoline-3,3'-isoxazolidin]-2-one derivatives has been developed *via* a transition metal- and base-free [3+2] cycloaddition reaction of isatin ketonitrone derivatives with β- nitrostyrene. The structures of these compounds were confirmed by NMR, HRMS, and single crystal X-ray. This method offers several advantages, including shorter reaction time, high yields, and a broad substrate scope. The synthesized compounds were evaluated for their in vitro antibacterial activities against two human pathogenic bacterial strains, *E. coli* and *S. aureus.* Among all the tested compounds, **11c** showed the highest potency, outperforming the standard antibiotic Gentamicin, with a MIC value of 20 μg ml-1. Structure-activity relationship studies (SARs) revealed that compound **11c**, having Cl- substituted styrene, possesses the most significant antibacterial activity. These spiro isoxazolidine derivatives exhibit promising antibacterial properties and favorable pharmacokinetic profiles, indicating their potential as viableantibacterialagents.

**Keywords:** [3+2] cycloaddition, Nitron, Isoxazolidines, Antibacterial study, Molecular Docking, DNA gyrase




***

# Click-Assembled Coumarin–BODIPY Conjugate as a Heavy-Atom-Free Photosensitizer for Combined Chemo-Photodynamic Therapy

**Abstract :**

Photodynamic therapy achieves spatial selectivity because its three components - photosensitizer, light and molecular oxygen- are individually benign. BODIPY dyes are attractive scaffolds but are intrinsically poor sensitizers, their efficient fluorescence outcompeting intersystem crossing. Heavy-atom substitution restores triplet formation at the cost of the emission required for image guidance and with the introduction of dark toxicity. We report **COU-BDP** , a heavy-atom-free BODIPY bearing two coumarin-substituted 1,2,3-triazoles installed by CuAAC, together with the matched phenyl analogue **PH-BDP** , which differs only at the terminal aryloxy group. Triplet population is engineered geometrically rather than electronically: DFT (CAM-B3LYP/6-311G(d,p)/CPCM) places the *meso* -aryl donor 69.5° from the dipyrromethene plane, and spin–orbit coupling calculations show the $S_1$-> $T_3$ channel to a charge-transfer triplet dominates (1.18 $cm^{-1}$) over locally excited channels (< 0.31 $cm^{-1}$), the signature of SOCT-ISC. Both conjugates retain substantial emission (Φ_F = 0.46 and 0.40), preserving imaging capability. Against MCF-7 cells, COU-BDP gave $IC_{50}$ = 54.7 μM in the dark and 7.4 μM under irradiation (phototoxic index 7.4), whereas PH-BDP fell only from 93.2 to 59.3 μM (index 1.6). Taking the quotient of the illuminated and dark potency ratios isolates a 4.69-fold strictly photodynamic contribution attributable to the coumarin unit. Caspase-3 activation rose 3.37-fold under illumination with half-maximal activation at 6.3 μM, matching the photodynamic $IC_{50}$ and establishing an apoptotic mechanism. Molecular docking identifies PARP-1 and topoisomerase IIα as candidate targets for the light-independent component.

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# Expedient fabrication of Eu doped ZnO/$SnO_2$ nanocomposite with enhanced photo degradation efficiency for hazardous contaminant by exposure to Methylene Blue colorant

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**Corresponding Author: amritapalai6@gmail.com**

## Abstract

In this study, Eu doped ZnO/$SnO_2$ nanocomposite samples with different $Eu^{3+}$ concentration (1.00-3.00 wt%) were synthesized by sol-gel method. Powder X-ray diffraction pattern confirmed the presence of both hexagonal ZnO and tetragonal $SnO_2$ simultaneously. The crystallite size and strain were calculated by using Debye Scherrer's method and Hall–Williamson method and it was found to be in the range of 11nm to 20 nm. Presence of functional group like stretching mode of Zn-O and Sn-O with the presence of stretching and bending vibration of absorbed water molecule (O-H) was confirmed by Fourier Transform Infra-red spectrometer. The FESEM images revealed the nanosheet structure of $Eu^{3+}$ doped ZnO/$SnO_2$ nanocomposite with a dimension of 45–75 nm. EDAX study shows the presence individual ion in the prepared sample. Luminescence studies have confirmed that $Eu^{3+}$ ions mainly occupy $Sn^{4+}$ sites in the $SnO_2$ part of the composite. The room temperature photoluminescence emission spectra show in the peak centered at 592 nm for the transition $^5D_0 \rightarrow {}^7F_1$ due to the presence of lanthanide ion. Other emissions peaks are observed due to zinc, tin and oxygen related defects. $Eu^{3+}$ doped nanocomposite is found to be suitable material with enhanced opto-electronic and luminescence properties and great applications in photocatalytic degradation of toxic environmental dye. The photocatalytic efficiency of the synthesized photocatalysts is evaluated by photodegradation of MB dye under visible light illumination. The presence of $Eu^{3+}$ ion in ZnO/$SnO_2$ enhance the degradation efficiency by the formation of Z- scheme heterojunctions between the ZnO and $SnO_2$. This allows the delay in recombination rate of the photogenerated electron/hole pairs due to the energy difference amongst the two oxides.

***Keywords:*** *Nanocomposite, Eu doped ZnO/SnO2, photocatalysis, Methylene Blue*

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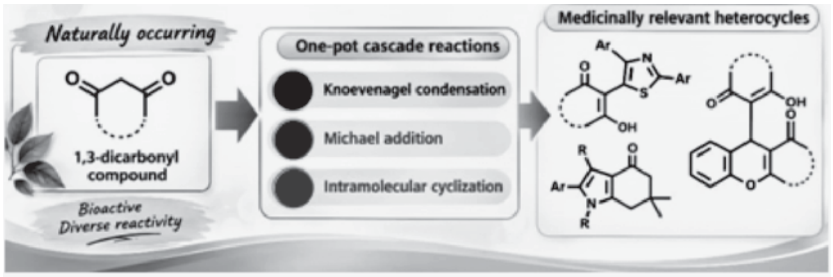
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# Harnessing the Unique Reactivity of 1,3-Dicarbonyls for the Synthesis of Medicinally Relevant Heterocycles Through One-pot Cascade Reactions

**Swadhin Swaraj Acharya, and Bibhuti Bhusan Parida**
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**Abstract:**
1,3-dicarbonyl compounds[1] are privileged class of molecules with natural occurrence, broad spectrum of bioactivities, and unique reactivity including both electrophilic as well as nucleophilic properties. Many popular name reactions such as Knoevenagel condensation, Biginelli reaction, Hantzsch reaction etc., and marketed medicines including felodipine, monastrol require 1,3-dicarbonyl compounds. As a consequence, research on 1,3-dicarbonyls became highly demanding. The multicomponent reactions (MCRs),[2] which also falls under cascade reaction is an active area of research in contemporary chemistry, since they meets the criteria of green chemistry and provides structural complexity in one-pot. We are therefore actively engaged in the synthesis of medicinally relevant heterocycles by harnessing the unique chemical reactivity of 1,3-dicarbonyls. As part of our on-going research we have prepared novel methodologies for the synthesis of functionalized thiazoles,[3] pyrroles,[4] and benzopyrans.[5,6]

**Keywords:** 1,3-dicarbonyl, cascade reactions, thiazole, pyrrole, benzopyran, bioactivity




**References:**
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6. S. S. Acharya, L. M. Barad, P. R. Rout, A. Bisoyi,B. B. Parida, *New J. Chem.*, **2025**, *49*, 12090-12101.

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# Fluorescence Quenching of Fluoroquinolone Drugs by Pyridine: Effect of Solvent

**Rakesh Kumar Sethi, Prabhati Padhan and Samarendranath Panda**
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**Abstract**

Fluorescence quenching of two fluoroquinolone drugs i.e. Lomefloxacin (LFX) and Levofloxacin (LVX) by pyridine has been investigated in organic solvents pyridine using steady state spectrofluorimeter in order to investigate the effect of dielectric constant and viscosity of the solvents on fluorescence quenching. It was observed that quenching is purely dynamic in low quencher concentration whereas quenching is transient one at higher quencher concentration. Both dielectric constant and viscosity coefficient of the solvents play an important role on the extent of quenching.

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# Aggregation-induced Emission Enhancement in Small Organic Molecules

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Aggregation-Induced Emission (AIE) is a distinctive photophysical phenomenon in which small organic molecules exhibit weak fluorescence in dilute solution but enhanced emission upon aggregation or in the solid state.[1,2] This behavior primarily results from the restriction of intramolecular motions, which suppresses non-radiative decay and promotes radiative emission. AIE-active molecules offer tunable optical properties, strong solid-state fluorescence, and structural versatility, making them valuable for applications in chemical sensing, bioimaging, environmental monitoring, and optoelectronic devices.[3,4]In this talk, I will briefly summarizes the fundamental mechanism and significance of AIE in small organic molecules, highlighting their potential in the development of advanced fluorescent materials.

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# Advances in the Total Synthesis of Indolactam Alkaloids

**Deepak Ranjan Mishra, Nilima Priyadarsini Mishra**

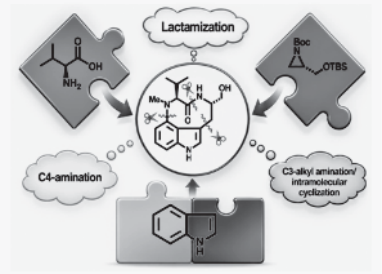
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**Email: drmishra.chem@gmail.com**

**Abstract :**

Indolactam is a structurally unique terpene indole alkaloid featuring a nine-membered lactam ring annulated to an indole core. This structurally unique class of indole alkaloid secondary metabolites is produced predominantly by actinomycetes, particularly *Streptomyces blastmyceticus* and related *Streptomyces* species, as well as marine cyanobacteria such as *Moorea producens*.[3-8] They constitute the biosynthetic core of several biologically important natural products, including indolactam V, indolactam I, teleocidin A2, lyngbyatoxin, pendolmycin and related metabolites.Indolactam alkaloids, owing to their diverse biological activities and challenging molecular architectures, have become attractive targets in synthetic organic chemistry. Their distinct and structurally complex indole-fused nine-membered lactam framework has stimulated the development of innovative synthetic strategies for efficient total synthesis. The key strategies employed to construct the characteristic nine-membered lactam ring, including intramolecular lactamization, intramolecular Heck coupling, and Lewis acid-catalyzed intramolecular cyclization.




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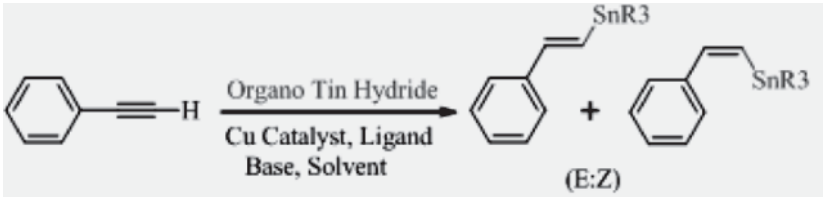
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# Copper-CatalyzedHydrostannylation of Alkynes: Ligand-Controlled Stereoselective Synthesis of Vinylstannanes

**Shivani Dehury, Gayatree Pradhan, Jaya Prakash Das**
**Department of Chemistry, Ravenshaw University, Cuttack, Odisha, India**

**Anstract :**

Hydrostannylation of alkynes represents a valuable strategy for the direct synthesis of vinylstannanes, which serve as versatile intermediates in organic synthesis. However, achieving efficient control over regio- and stereoselectivity remains a significant challenge, particularly in the hydrostannylation of unsymmetrical alkynes. In the present study, we investigate a copper-catalyzedhydrostannylation methodology for the synthesis of vinylstannanes using tributyltin hydride as the stannylating reagent, with particular emphasis on the influence of ligand architecture on stereoselectivity.




Scheme: Copper-catalyzed hydrostannylation of alkynes

investigations using CuCl in combination with different ligands demonstrated efficient conversion of the alkyne substrate, while significant variations in the E/Z ratio were observed. CuCl/1,10-phenanthroline and CuCl/$PCy_3$ systems afforded >95% crude yield with pronounced preference for the Z-isomer, giving E/Z ratios of approximately 37:63 and 13:87, respectively. In contrast, the use of $PPh_3$ resulted in a nearly 60:40 E/Z ratio. These results demonstrate that the ligand environment strongly influences the stereochemical outcome of copper-catalyzedhydrostannylation. Further optimization of the catalyst, ligand, base, solvent, and reaction parameters is being pursued to improve stereoselectivity and establish a broader substrate scope. The optimized methodology will subsequently be evaluated with diverse aryl, heteroaryl, and aliphatic alkynes, followed by exploration of the synthetic utility of the resulting vinylstannanes. The details will be discussed in the poster.

***Keywords:*** Hydrostannylation; Copper catalysis; Vinylstannanes; Stereoselectivity; Ligand effects.

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# Pot-, Atom, and Step-Economic (PASE) Synthesis of Functionalized Pyrans From 1, 3- dicarbonyls.

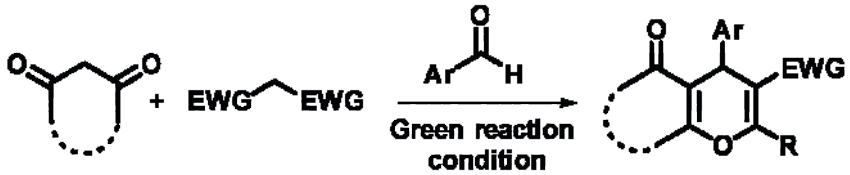
**Subhakalyani Nayak, Swadhin Swaraj Acharya, Rudranarayan Sutar, Debiprasad Panda and Bibhuti Bhusan Parida**

***Organic Synthesis Laboratory, P. G. Department of Chemistry, Berhampur University, Bhanja Bihar, Odisha-760007***

**Abstract:**

1,3-dicarbonyls1 are unique molecular units with natural occurrence, bioactivity, and interesting chemical properties; they possess both electrophilicity, and nucleophilicity. They find applications in many name reactions and the synthesis of drugs. Consequently, it has become an active area of research. Like the 1,3-dicarbonyls, 4*H*-pyrans2,3 are privileged molecules with promising bioactivities. The multicomponent reactions (MCRs),4,5,6 is an active area of research in contemporary chemistry, since they fulfil the criteria of green chemistry and provides complex molecules in one-pot. We therefore have synthesized the fused pyrans derived from natural products utilizing the unique chemical property of 1,3-dicarbonyls.

**Keywords:** 1,3-dicarbonyl, cascade reactions, pyran, bioactivity, multicomponent reactions.




**References:**

1. S. S. Acharya, D. Samantaray, C. Sibakrishna, B. B. Parida, *ChemistrySelect*, **2025**, *10*, e202403416.
2. S. S. Acharya, P. R. Rout, L. M. Barad, J. Dansana, A. Gadtya, B. R. Meher, B. B. Parida, *Org. Biomol. Chem.*, **2025**, *23*, 8465-8473.
3. S. S. Acharya, L. M. Barad, P. R. Rout, A. Bisoyi, B. B. Parida, *New J. Chem.*, **2025**, *49*, 12090-12101.
4. S. S. Acharya, P. R. Rout, R. Sutar, C. Pradhan, B. B. Parida, *Adv. Synth. Catal.*, **2025**, *367*, e202500184.
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6. S. S. Acharya, R. Sutar, G. P. Mishra, B. B. Parida, *Org. Biomol. Chem.*, **2026**, 24, 5064-5077.

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# Eco-Friendly Adsorption of Methyl Orange dye using Neem Leaves (*Azadirachta indica*)

**Soumyaranjan Das Mohapatra, Subhashree Samal, Subhamkar Nayak and Niranjan Biswal**

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**Abstract :**

This study invstigates an eco-friendly approach for the removal of methyl orange (MO) dye from aqueous solutions using neem leaves (*Azadirachta indica*) as a natural adsorbent. The neem leaves were collected, washed, dried, and powdered before being utilized in batch adsorption experiments. The effects of various operational parameters, including dye concentration (1–150 mg/L), pH (1–7), adsorbent dosage (0.05–0.15 g), contact time (30–180 minutes) and were systematically examined.

The results indicated that adsorption efficiency increased with contact time and reached a maximum of 72.96% at 90 minutes for $NL_4$ adsorbent**,** after which a slight decrease was observed. Maximum adsorption occurred under acidic conditions, particularly at pH 1.5**,** due to enhanced electrostatic interactions. An increase in adsorbent dosage improved dye removal efficiency, while higher dye concentrations led to reduced adsorption due to saturation of active sites. Among the prepared adsorbents, $NL_4$ exhibited the highest adsorption performance**.**

These findings demonstrate that neem leaves powder is a low-cost, sustainable, and effective adsorbent for dye removal from water, with potential applications in environmentally friendly water treatment systems. The adsorption process of methyl orange onto neem leaves powder was found to follow pseudo-second-order kinetics and the Langmuir isotherm model, respectively.

**Keywords:** *Neem Leaves; Methyl Orange; Adsorption; Water pollution abatement*

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# Investigation of chemical composition and yield of extracted essential oils from *Cymbopogon citratus*, *Citrus sinensis*, and *Curcuma longa*

**Afreen Banu, Madhusmita Choudhury, Harapriya Sahu and Niranjan Biswal ***

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Essential oils are complex mixtures of organic compounds with significant applications in cosmetics, pharmaceuticals, and the food industry. The aim of this research is to analyse the chemical composition and evaluates the yield of extracted essential oils (EOs) from different forms of *Cymbopogon citratus*, *Citrus sinensis*, and *Curcuma longa*. The EOs were extracted by using steam distillation at a temperature of 100 °C for approximately 4 h. The chemical composition was analysed using Liquid Chromatography–Mass Spectrometry (LC–MS), High-Performance Liquid Chromatography (HPLC), and Nuclear Magnetic Resonance (NMR). From HPLC, dry lemongrass showed citral at a concentration of 38.47 % whereas turmeric showed demethoxycurcumin and bisdemethoxycurcumin at concentration of 46.67 % and 39.71 % respectively. LCMS showed a major peak in the case of dried orange oil, which indicates the presence of 15.60 % limonene. The highest yield was obtained from dried orange peels (3.43 % v/w), followed by dried lemongrass (2.13 % v/w).

**Keywords:** *Steam distillation; citral (geranial and neral); limonene; curcumin; demethoxycurcumin (DMC)*

***

# Biological importance of Indanes, Chromans and their Synthetic Approach

**Dr. Sagarika Behera, Asst. Professor,**
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## Abstract:

Carbocycles such as indanes, chromans, and indenes are important motifs present in several pharmaceutical drugs and their derivatives have exhibit biological activities including antitumor, anti-hypercholesterolemic, antiallergic, anticonvulsant, fungicidal, and antimicrobial activities. 4-methoxy-1,1-indane is a well-known precursor for the synthesis of anti-cancer drugs.Derivatives of indanes have wide application in the field of material science such as a superconductor and used in organic vapour sensing material in OLED (like 1,3-Bis(4- imino-3-hydroxybenzoic acid) indane used by Langmuir-Blodgett (LB) thin film deposition technique to sensing gas. Due to their wide importance, the development of a new synthetic approach towards their synthesis is the key of research interest. There are various traditional and transition metal catalyzed methods that have been reported. This report mainly focuses on acid-catalysed synthesis of indanes and chromanol derivatives. Chroman (dihydrobenzopyran) is a challenging moiety found in important biologically active compounds such as Clusifoliol, Vitamin E and its derivatives known as pro-oxidant. Vitamin E is an antioxidant, also It represents itself as a signaling molecule, used as a regulation of gene expression, in the prevention of cancer and atherosclerosis.

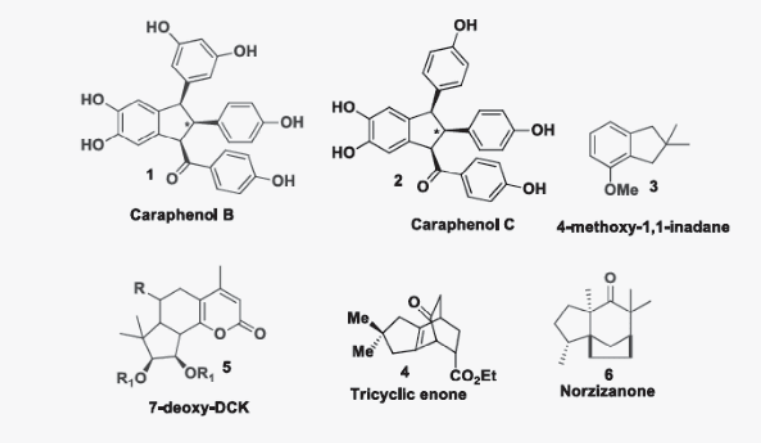



Figure: Biologically active indane derivatives

**Keywords**: Indanes, Chromanols, Acid-catalysed, Cyclization,Tocopherol

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# Heterocyclic Schiff-Base Polymeric Resins: Synthesis, Characterization and Applications in Toxic Metal Sensing and Arsenic Remediation

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**Abstract**

The contamination of water resources by toxic heavy metals and arsenic species has emerged as a major environmental concern, creating an urgent need for efficient, selective and reusable materials for their detection and removal. In this context, the present research focuses on the design and development of functionalized polymeric Schiff-base resins incorporating heterocyclic donor sites for selective metal-ion recognition and environmental remediation. Three heterocyclic Schiff-base systems based on **6-ethoxy-2-aminobenzothiazole, 2-aminobenzimidazole and 2-aminopyridine** have been investigated for their potential to interact with toxic metal ions, particularly **Cu(II), Hg(II) and Pb(II)**. The synthesized polymeric materials are being systematically characterized using spectroscopic, thermal and morphological techniques, including FT-IR, UV–Vis, NMR, TGA, SEM–EDX and XPS, to establish their structural features and surface characteristics.

The research further explores the application of these functionalized resins in **metal-ion sensing and adsorption**, with particular emphasis on the development of Cu(II)- and Fe(III)-loaded polymeric ligand exchangers for the selective uptake of **As(V) and As(III)** from aqueous media. The sensing behaviour is being evaluated with respect to selectivity, sensitivity, response characteristics, pH dependence and interference from competing ions, while adsorption studies include the effects of contact time, pH and initial contaminant concentration. Kinetic, equilibrium-isotherm and thermodynamic investigations are being undertaken to elucidate the adsorption mechanism, together with studies on regeneration, reusability and selectivity. The applicability of the developed materials is also being examined using real water samples relevant to arsenic and heavy-metal contamination in Odisha and India. The study aims to establish a multifunctional polymeric platform integrating **selective sensing, adsorption and separation**, thereby contributing to the development of practical materials for monitoring and remediation of toxic metal and arsenic contamination in water.

**Keywords**

Schiff-base resins; Heterocyclic ligands; Metal-ion sensing; Arsenic removal; Water remediation

***

# Design and Development of Schiff-Base Functionalized Magnetic Nanopolymeric Composites for Colorimetric Sensing and Separation of Toxic Metal Ions from Water

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**Buxi Jagabandhu Bidhyadhar Autonomous College, Bhubaneswar**
**Corresponding Author- maildebasismohanty@gmail.com**

## Abstract

The presence of toxic metal ions in aquatic systems poses a serious environmental challenge owing to their persistence, bioaccumulation and potential adverse effects on living organisms. The development of multifunctional materials capable of both rapid detection and efficient removal of toxic metal ions is therefore of considerable importance. The present study focuses on the design and development of **Schiff-base functionalized magnetic nanopolymeric composites** for the selective colorimetric sensing and separation of toxic metal ions from aqueous media. Two structurally related nanocomposites, **NC-1 ($Fe_3O_4$ @Chitosan–Salicylaldehyde Schiff Base)** and **NC-2 ($Fe_3O_4$ @Chitosan–5-nitrosalicylaldehyde Schiff Base)**, have been designed to investigate the influence of nitro substitution on the physicochemical, sensing and adsorption characteristics of the resulting materials.

The incorporation of $Fe_3O_4$ nanoparticles provides magnetic responsiveness and facilitates rapid separation and recovery of the adsorbent, while Schiff-base functionalization introduces coordination-active sites for interaction with toxic metal ions. Particular attention is being given to **Cr(VI) and Cd(II)** as target contaminants. The synthesized materials are being systematically characterized using FT-IR, UV–Visible spectroscopy, XRD, SEM/TEM-EDX, TGA, BET, VSM and XPS techniques to establish their structural, morphological, thermal, surface and magnetic properties. Their colorimetric response towards target metal ions is being investigated with respect to sensitivity, selectivity, response time, concentration dependence and the influence of competing ions.

In parallel, batch adsorption studies are being undertaken to evaluate the effects of pH, contact time, adsorbent dosage and initial metal-ion concentration. Adsorption kinetics, equilibrium isotherms and thermodynamic parameters are being examined to understand the adsorption mechanism. The magnetic character of the composites is further exploited for facile solid–liquid separation, while regeneration and reusability studies are being carried out to assess their practical applicability. Comparative evaluation of NC-1 and NC-2 is expected to provide insight into the role of **electron-withdrawing nitro substitution in tuning Schiff-base functionality, metal-ion recognition and adsorption behaviour**. The study ultimately aims to develop a multifunctional, magnetically recoverable nanopolymeric platform that integrates **colorimetric detection with efficient separation of toxic metal ions**, with potential application in monitoring and remediation of contaminated water.

**Keywords**

Magnetic nanocomposite; Schiff-base polymer; Colorimetric sensing; Toxic metal ions; Arsenic remediation

***

# Physicochemical Investigation of L-Histidine-Valine, and L-Serine in Aqueous Chlortetracycline Hydrochloride Solutions

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**Abstract :**

The Physicochemical behaviour of the biologically significant amino acids L-histidine, L-valine, and L-serine in aqueous chlortetracycline hydrochloride solutions was investigated over a selected temperature range using measurement of density (ρ), apparent molar volume (Vϕ), viscosity (η), ultrasonic velocity (U), and partial isentropic compressibility (Kϕ, s). In addition, the transfer properties of the amino acids and the Jones-Dole viscosity coefficients (A and B) were evaluated to elucidate the nature of solute-solute and solute-solvent interactions. The experimental results reveal that the variation in density, ultrasonic velocity apparent molar volume, viscosity, and partial isentropic compressibility is governed by the combined effects of hydrogen bonding, ion-dipole interactions, electrostrictive hydration, and hydrophobic interactions between the amino acids and chlortetracycline hydrochloride molecules. Positive transfer parameters together with favorable B-coefficient values indicate enhanced hydration and stronger solute-solvent association, promoting structure-making behaviour of the aqueous medium. Conversely, thermal agitation at higher temperature weakens intermolecular interactions, leading to partial structure-breaking behaviour and reduced hydration. Among the investigated amino acids, differences in side-chain functionality significantly influence the extent of molecular association and the resulting structural organization of the solution, providing valuable insights into amino acid-drug interactions relevant to pharmaceutical and biological systems.

Keywords: L-histidine, L-valine, and L-serine, chlortetracycline hydrochloride, ion-dipole interactions, hydrogen bonding

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# Uses of Supramolecular Polymers in DNA Fragments

**Rameez Hasan Raza, Guruprasad Dash**

## Abstract

Supramolecular polymers are dynamic polymeric materials formed through reversible and non-covalent interactions such as hydrogen bonding, π–π stacking, electrostatic interactions, metal–ligand coordination, and host–guest recognition. Their unique combination of structural adaptability, self-assembly, and reversible interactions makes them highly promising for applications involving DNA fragments and nucleic-acid-based systems. Supramolecular polymers can interact with DNA through electrostatic attraction, hydrogen bonding, base recognition, and aromatic stacking, enabling controlled DNA binding, condensation, stabilization, and transport. These materials have potential applications in gene delivery, DNA sensing, molecular recognition, biosensing, and the protection of DNA against enzymatic or environmental degradation. Their dynamic nature also allows responsive interactions with DNA under changes in pH, temperature, ionic strength, or the presence of specific biomolecules. Furthermore, supramolecular polymer–DNA assemblies can serve as functional platforms for constructing nanoscale architectures and developing advanced biomedical materials. This topic highlights the fundamental principles of supramolecular polymer formation, their interactions with DNA fragments, and their emerging applications in biotechnology, diagnostics, drug delivery, and nanomedicine.

**Keywords:** Supramolecular polymers, DNA fragments, Self-assembly, Molecular recognition, DNA binding, Gene delivery, Biosensing, Nanomedicine.

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# Molecular Warriors: The Chemistry Behind Anticancer Drugs"

**Anuradha Nanda[1],BebiMohapatra[1], Subhalaxmi Dehury**
**Ranee Rout, Guruprasad Dash**

**Abstract:**

Cancer is a complex disease characterized by uncontrolled proliferation and division of abnormal cells, making the development of effective and selective therapeutic agents a major challenge. **Anticancer drugs act as molecular warriors by exploiting specific chemical interactions with DNA, proteins, enzymes, microtubules, and cellular signaling pathways.** This poster highlights the fundamental role of chemistry in the design, synthesis, structural optimization, and mechanism of action of representative anticancer drugs. Particular emphasis is placed on **cisplatin**, a platinum-based coordination complex that undergoes ligand substitution and forms platinum–DNA adducts, and **5-fluorouracil (5-FU)**, a fluorinated pyrimidine analogue that interferes with nucleotide metabolism and inhibits DNA synthesis. Other important therapeutic classes, including anthracyclines, taxanes, and targeted kinase inhibitors, are discussed in relation to their characteristic molecular structures and biological targets. The relationship between **molecular structure and biological activity (SAR)** is examined to demonstrate how functional groups, molecular geometry, electronic properties, and specific intermolecular interactions influence drug potency and selectivity. Characterization techniques such as **XRD, FTIR, UV–Vis, NMR, MS and XPS** provide essential information about molecular structure and physicochemical properties. The poster further presents major mechanisms including DNA damage, enzyme inhibition, disruption of cell division, apoptosis, and signal-transduction blockade. Understanding these molecular and chemical principles provides a foundation for developing **more selective, effective, and safer anticancer therapies**, including targeted, combination, and personalized treatment strategies.

**Graphical Abstract**

**Keywords:**Anticancer drugs; Cisplatin; 5-Fluorouracil; Molecular structure; SAR; DNA damage; Drug design; Targeted therapy; Medicinal chemistry.

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# Voltammetric Determination of Nicotine Using a Graphene-Modified Glassy Carbon Electrode

**Sardaprasad satapathy[1],Debadatta Moharana[1], Guruprasad Dash[1a]**

**Abstract**

Nicotine is an important alkaloid present in tobacco products, and its rapid and sensitive determination is significant for tobacco quality control, environmental monitoring, and health-related studies. In the present work, a graphene-modified glassy carbon electrode (Graphene/GCE) is proposed as an electrochemical sensing platform for the voltammetric determination of nicotine. Graphene was selected as an electrode-modifying material because of its high surface area, excellent electrical conductivity, and favorable electron-transfer characteristics. The modified electrode is investigated using cyclic voltammetry (CV) to evaluate the electrochemical behavior of nicotine and the enhancement provided by the graphene layer. Differential pulse voltammetry (DPV) is employed for quantitative determination after optimization of experimental parameters such as supporting electrolyte, pH, graphene loading, and instrumental conditions. The graphene-modified electrode is expected to provide an enhanced oxidation response toward nicotine compared with the bare glassy carbon electrode owing to the increased electroactive surface area and improved interfacial electron-transfer kinetics. Analytical performance is evaluated in terms of linearity, sensitivity, limit of detection, reproducibility, selectivity, and stability. The proposed Graphene/GCE platform offers a simple, rapid, and potentially low-cost approach for voltammetric nicotine determination and demonstrates the potential of graphene-based nanomaterials for electrochemical sensing applications. Interference studies demonstrated high selectivity for nicotine in the presence of common co-existing species such as ascorbic acid, uric acid, and glucose. The sensor was successfully applied to real-sample analysis, including commercial e-cigarette refill liquids and human urine matrixes, yielding recovery rates between 96.5\% and 103.2\%. Overall, the nanocomposite platform offers a robust, cost-effective alternative to conventional chromatographic methods for routine nicotine monitoring in environmental, forensic, and biological contexts.

**Keywords:** Nicotine; Graphene; Glassy carbon electrode; Voltammetry; Differential pulse voltammetry; Electrochemical sensor.

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# Nanochemistry: Principles, Applications and Emerging Perspectives

**Balaram Jena[1], Guruprasad Dash**

**Abstract**

Nanochemistry is an interdisciplinary branch of chemistry concerned with the synthesis, characterization, properties, and applications of materials with dimensions typically ranging from 1 to 100 nm. At the nanoscale, materials exhibit unique physicochemical properties arising from their high surface-to-volume ratio, quantum confinement, surface energy, and size-dependent electronic and optical behavior. These characteristics have enabled the development of advanced nanomaterials with applications across chemistry, materials science, medicine, environmental science, energy, and catalysis. Nanochemistry encompasses diverse materials, including metal and metal oxide nanoparticles, carbon-based nanomaterials, graphene, carbon nanotubes, quantum dots, nanocomposites, and semiconductor nanostructures. Various approaches, such as sol–gel processing, precipitation, hydrothermal synthesis, chemical reduction, microwave-assisted synthesis, and green synthesis, are employed to control particle size, morphology, composition, and surface properties. Advanced characterization techniques including X-ray diffraction, electron microscopy, spectroscopy, and surface analysis are essential for understanding nanoscale structure–property relationships. Nanochemical materials have demonstrated considerable potential in photocatalytic pollutant degradation, electrochemical sensing, drug delivery, antimicrobial applications, energy conversion and storage, and water purification. Despite these advances, challenges related to controlled synthesis, aggregation, scalability, environmental impact, toxicity, and long-term stability remain important areas of research. Continued development of sustainable synthesis strategies and multifunctional nanomaterials is expected to expand the role of nanochemistry in addressing emerging technological and environmental challenges.

**Keywords:**Nanochemistry; Nanomaterials; Nanoparticles; Graphene; Nanocomposites; Nanocatalysis; Green synthesis; Environmental applications.

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# Molecular Dynamics Simulation in Chemistry: A Computational Approach to Understanding Molecular Motion and Interactions

**MukeshMohapatra[1], Guruprasad Dash [1a]**

## Abstract

Molecular Dynamics (MD) simulation is a powerful computational technique used to investigate the structure, motion, and interactions of atoms and molecules at the molecular level. In MD simulations, the behavior of interacting particles is described by classical equations of motion, generally using an appropriate force field to calculate potential energies and interatomic forces. By solving these equations over successive time steps, the trajectories of atoms and molecules can be generated and analyzed to obtain detailed information about molecular structure, diffusion, thermodynamic properties, intermolecular interactions, and dynamic processes. Molecular Dynamics provides a microscopic perspective that is often difficult to obtain through conventional experimental techniques. For example, simulations of liquid water can reveal molecular movement, hydrogen-bonding interactions, structural rearrangements, and diffusion behavior over time. The method has wide applications in physical chemistry, materials science, nanotechnology, biochemistry, drug discovery, catalysis, and energy-related research. It is also increasingly valuable for studying complex chemical systems, designing advanced materials, and predicting molecular properties before experimental investigation. Overall, Molecular Dynamics Simulation serves as an important bridge between theoretical chemistry, computational modeling, and experimental research. With advances in computational power and simulation methodologies, MD has become an essential tool for understanding molecular-level phenomena and guiding the development of new chemical and functional materials.

**Keywords:** Molecular Dynamics, Computational Chemistry, Molecular Simulation, Force Field, Molecular Motion, Intermolecular Interactions, Molecular Trajectory, Computational Modeling.

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# $H_2$ : A sustainable energy solution

**Pritimayee Sahoo, Biswomitra Sahoo, Soumya Suravi**

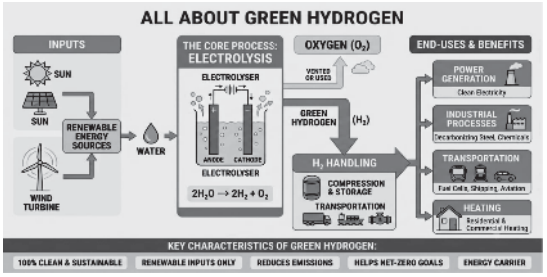
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**Abstract:**

Green hydrogen is a clean and sustainable energy carrier produced mainly by splitting water into hydrogen and oxygen through electrolysis using renewable energy such as solar, wind and hydropower. Because it can be produced without the direct use of fossil fuels, green hydrogen has the potential to reduce carbon emissions and support the transition towards a low-carbon energy system. In India, it can be used in fertilizer production, petroleum refining, steel manufacturing, heavy transportation, shipping, power generation and other hard-to-decarbonize industries. It can also be converted into derivatives such as green ammonia and green methanol. Safe and efficient storage and transportation are important for its large-scale use; hydrogen can be stored as compressed gas or liquid and transported through pipelines, tankers and other dedicated infrastructure. India's National Green Hydrogen Mission aims to develop domestic production, technology, infrastructure and a strong green-hydrogen ecosystem, while promoting research, innovation and industrial applications. Future development of green hydrogen will focus on improving electrolyser efficiency, developing low-cost catalysts and membranes, advanced materials, fuel cells, hydrogen storage and transportation technologies, hydrogen production from biomass, and seawater electrolysis. Research is also exploring safer, more durable and economical materials and technologies to make hydrogen production and utilization more efficient and scalable. With continued research and technological development, green hydrogen can contribute to cleaner industries, energy security, renewable-energy integration and a more sustainable future for India.

**Graphical Abstract:**




**Keywords:**

Green Hydrogen, Water Electrolysis, Renewable Energy, Carbon Emission Reduction, Green Ammonia, Green Methanol, Hydrogen Storage, Hydrogen Transportation, National Green Hydrogen Mission, Electrolyser Technology, Fuel Cells, Sustainable Future.

**Reference:**

1. Hydrogen and Fuel Cells: Emerging Technologies and Applications — Bent Sørensen & Giuseppe Spazzafumo, 2018.
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# Applications of Organometallic Complexes in Medicinal Chemistry

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**Abstract**

Organometallic chemistry has emerged as a promising area of medicinal chemistry owing to the distinctive structural, electronic, and biological properties of metal-containing compounds. Unlike conventional organic drugs, organometallic complexes combine the reactivity of organic ligands with the unique characteristics of metal centres, providing opportunities for developing novel therapeutic agents. This article reviews the potential applications of organometallic complexes in medicinal chemistry, with particular emphasis on their roles in anticancer, antimicrobial, and diagnostic applications. Transition-metal complexes based on metals such as ruthenium, iron, platinum, gold, and cobalt have attracted considerable attention because of their diverse mechanisms of biological action, including interaction with biomolecules, generation of reactive species, inhibition of enzymes, and modulation of cellular signalling pathways. Organometallic compounds can also be designed to improve target selectivity, cellular uptake, and controlled biological activity through appropriate modification of their ligands and metal centres. In particular, metal-based compounds have demonstrated considerable potential as alternatives or complements to conventional therapeutic agents. Recent developments in organometallic drug design, targeted delivery, and photoactivated therapeutic systems further illustrate the expanding scope of this field. Despite these advances, issues related to toxicity, stability, selectivity, and pharmacokinetic behaviour remain important challenges. Continued integration of organometallic chemistry, medicinal chemistry, and molecular biology may therefore contribute to the development of safer and more effective metal-based therapeutic agents.

**Keywords:** Organometallic complexes, medicinal chemistry, metal-based drugs, transition metals, anticancer agents, antimicrobial agents, drug design.

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# Interfacial Charge Transfer in B-Dopedg-C3N4/mixed phase TiO2 p-n Heterojunction Photocatalyst for the degradation of Antibiotics under visible light

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**Abstract**

Ciprofloxacin (CIP) and other harmful pharmaceutical substances must be rapidly removed from water, which is still a serious environmental problem. An efficient visible-light-driven B-doped g-$C_3N_4$/$TiO_2$ p-n heterojunction photocatalyst was developed in this work, aiming at improving degradation performance. The electronic structure of g-$C_3N_4$ had been modulated by doping boron, increasing charge mobility and expanding its visible light absorption. By coupling B-g-$C_3N_4$ with spinel $TiO_2$, a stable p-n heterojunction was created, which remarkably enhanced interfacial charge separation through internal electric field formation. Systematic photocatalytic experiments has indicated that this heterojunction exhibited much higher degradation efficiency toward ciprofloxacin under visible light in comparison with its counterparts. Its enhanced performance had been illustrated based on the internal electric field at the interface of the p-n heterojunction, with the synergistic effect of boron doping, which would promote the directional charge migration and increase charge carrier lifetime. This study proposes a feasible approach toward the development of high-performance heterojunction photocatalysts for the efficient removal of newly identified pharmaceutical contaminants.

**Keywords:-** B-Dopedg-$C_3N_4$/$TiO_2$, p-n heterojunction, ciprofloxacin, photocatalytic degradation.

**Acknowledgement: -** The work is supported by Extra-mural research funding under MRIP-2023 Chemistry (23EM/CH/14).

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# Harnessing Naturally Occurring 1,3-dicarbonyls for the One-pot Domino Synthesis of Medicinally relevant Functionalized Pyrans

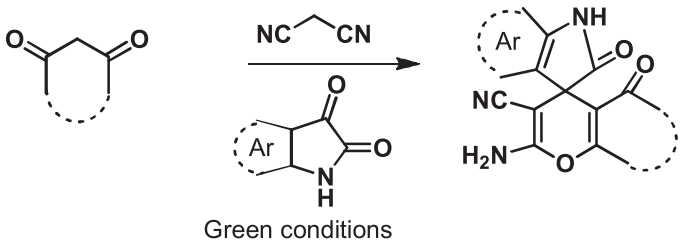
**Debiprasad Panda**,SwadhinSwaraj Acharya,SubhakalyaniNayak,RudranarayanSutar,

and Bibhuti Bhusan Parida*

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**Abstract:** 1,3-dicarbonyls[1]represents an important class of molecules owing to their natural occurrence (curcumin, lyciumines A, ginderdione, lawsone), impressive biological and medicinal profile (anticancer, antimalarial, antifungal, antimicrobial, antitumor). Alongside, they possess interesting chemical feature which makes them a suitable candidate for the synthetic chemists. Their electrophilic and nucleophilic properties are helpful for the synthesis of fused and spiroheterocycles. Likewise, the pyran[2,3] is a celebrated scaffold owing to their occurrence in numerous natural products including tomentosa A, tomentosa B, rhodomyrtone, rhodomyrtosone C, myrtucommuloneC, myrtucommulone E, cudraflavone B, cyclochampedol, millewanin G etc. Therefore they are highly important in drug discovery. Contemporary organic synthesis demand greener synthetic approaches that minimize the overall steps, by avoiding the toxic chemicals. In this context, the multicomponent reactions[4,5] are getting popularity. Therefore, we report the multicomponent synthesis of fused, and spiropyrans involving the 1,3-dicarbonyl compounds.

**Keywords:** 1,3-dicarbonyl, cascade reactions, pyran, bioactivity, multicomponent reactions




**References:**

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   S. S. Acharya, B. K. Guin, B. B. Parida, *J. Org. Chem.*, **2025**, *90*, 2717–2727.

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# Synthesis of $NH_2$ -MIL-88B(Fe) as a Promising Iron-Based MOF for Photocatalytic Environmental Applications

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Water pollution caused by organic dyes, pharmaceutical residues, antibiotics, and toxic heavy metals has emerged as a significant environmental concern, creating an urgent need for efficient and sustainable remediation technologies. Metal–organic frameworks (MOFs) have attracted considerable attention as versatile functional materials because of their high porosity, large surface areas, tunable structures, and adjustable chemical properties. Among various MOFs, iron-based frameworks, particularly $NH_2$ -MIL-88B(Fe), have shown considerable potential for photocatalytic and environmental applications owing to their visible-light responsiveness, iron-containing active centres, and amino-functionalized framework.

In the present study, $NH_2$ -MIL-88B(Fe) MOF was synthesized through a solvothermal approach using an iron salt and 2-aminoterephthalic acid as the metal precursor and organic linker, respectively. The synthesized material was analyzed by powder X-ray diffraction (PXRD), which showed prominent reflections at $2\theta \approx 9.2°$, 10.3°, 13.1°, 16.7°, 18.5°, 20.7°, and 29.0°. The observed reflections are consistent with the characteristic diffraction pattern reported for $NH_2$ -MIL-88B(Fe), indicating the successful formation of the targeted MOF structure.

The presence of redox-active iron centres in the framework can facilitate electron-transfer processes involved in photocatalytic reactions, while amino functionalization can enhance the interaction of the MOF with target pollutants and influence its electronic properties. These features make $NH_2$ -MIL-88B(Fe) an attractive candidate for photocatalytic environmental remediation. The present preliminary structural study provides a foundation for further physicochemical characterization and evaluation of its photocatalytic performance toward environmentally relevant pollutants. Further studies are currently underway to investigate its properties and potential applications in pollutant degradation and advanced oxidation processes.

**Keywords :** $NH_2$ -MIL-88B(Fe); MOF; solvothermal synthesis; PXRD; photocatalysis.

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# Waste-to-Wealth through Gasification: A Sustainable Approach to Energy Recovery

**Pravasini Tripathy[1],Sarojini Das[1], Priyambada Priyadarsini[1], Guruprasad Dash[1a]**

## Abstract

The rapid generation of municipal solid waste, agricultural residues, and industrial wastes has created significant environmental challenges while simultaneously increasing the demand for sustainable energy resources. Gasification offers a promising waste-to-energy pathway by converting carbonaceous waste materials into a combustible synthesis gas (syngas), primarily composed of carbon monoxide, hydrogen, methane, and carbon dioxide, under controlled conditions with limited oxygen or steam. This technology provides an opportunity to transform otherwise underutilized waste into useful energy carriers while reducing the volume of waste requiring disposal. The composition and quality of syngas depend strongly on feedstock characteristics, gasification temperature, gasifying agent, reactor configuration, and operating conditions. The produced syngas can be utilized for heat and electricity generation or further processed for the production of fuels and valuable chemicals. Gasification can also contribute to resource recovery, reduction of greenhouse-gas emissions, and improved waste-management efficiency when appropriately designed and operated. However, challenges associated with tar formation, feedstock heterogeneity, process optimization, emissions control, ash management, energy efficiency, and economic viability remain important considerations. Advances in reactor design, catalytic gasification, emission-control technologies, and integration with renewable energy systems are improving the prospects of this technology. Thus, waste gasification represents a potential circular-economy approach in which waste is converted into energy and valuable products, supporting sustainable resource utilization and reducing dependence on conventional fossil fuels.

**Keywords:** Waste gasification; Waste-to-energy; Syngas; Sustainable energy; Biomass; Circular economy; Energy recovery; Waste management.

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# Forever Chemicals, Forever Problems: The PFAS Challenge in Indian Waters

**PravasiniTripathy, SarojiniDas,PriyambadaPriyadarsini and Dr. Jaykishon Swain**

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## Abstract

Per- and polyfluoroalkyl substances (PFAS), dubbed “forever chemicals” for their extreme persistence, are emerging contaminants of global concern. Widely used in non-stick coatings, firefighting foams, and food packaging, PFAS accumulate in water, soil, and living organisms, with links to thyroid disorders, immune suppression, and certain cancers. This presentation provides a critical overview of PFAS contamination in Indian water systems, highlighting sources, transport pathways, and exposure risks. Analytical techniques such as LC-MS/MS, HPLC, and high-resolution mass spectrometry for PFAS detection and quantification are discussed. The effectiveness of treatment technologies—including activated carbon, ion exchange, and advanced oxidation—is evaluated. Regulatory gaps in India and the need for comprehensive monitoring frameworks are emphasised. The current study calls for urgent scientific and policy interventions to address this silent chemical crisis and protect public health and environmental integrity.

**Keywords:** PFAS, Water Pollution, Advanced Oxidation Process

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# Micellar and solvent effect on kinetics and mechanism of oxidation of Diclofenacand Aceclophenac, NSAID by copper (III) period ate complex.

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The kinetics of oxidation of two nonsteroidsantiinflammatory drugs aceclophenac and Diclofenac in aqueous alkaline medium has been studied in temperature range 293 K to 313K spectrophotometrically. The kinetics of electron transfer to (DPC) diperiodatocuprate (III) from nonsteroid, antiarthritis drugs DFS and ACE follows a zero order reaction with respect to DPC and nearly unity order dependence on [DFS]/[ACE] and dependence on the [$OH^-$]. The diperiodatocuprate (III) is a powerful oxidising agent in alkaline medium,monoperiodatecuprate(III) [$Cu(H_2IO_6)(H_2O)_2$] is considered to be active species . The derived rate law and proposed mechanism supports stoichiometry of the oxidation reaction Cu (III) and drug and formation of measure product such as [2- (2, 6-dichloro-phenyl amino) phenyl] methanol. The product was confirmed by GCMS and 1H NMR spectra. The moderate values of activation parameters favor the electron transfer process; the low value of activation enthalpy indicates the stability of the complex. The high value of negative entropy suggests the rigid transition state. Both enthalpy and entropy control the stabilities of transition state. The kinetics of redox reaction by DFS/ACE in alkaline medium is catalyzed by SDS for DFS and independent in case of ACE. But both show rate retardation in presence of neutral micelles TX-100. Hence SDS is an excellent catalyst as compared to TX-100 for the above redox reaction. The aprotic solvent DMSO accelerates the redox process in DFS and ACE. Howeverprotic solvent ($CH_3OH$) shows no effect on the redox reaction. Hence the reaction is best catalyzed in DMSO medium.

**Key Word:** diclofenac,diperiodatocuprate,TX -100,aceclofenac drug DFS/ ACE with Cu (III)/Cu (II) indicating outer-sphere electron transfer mechanism.

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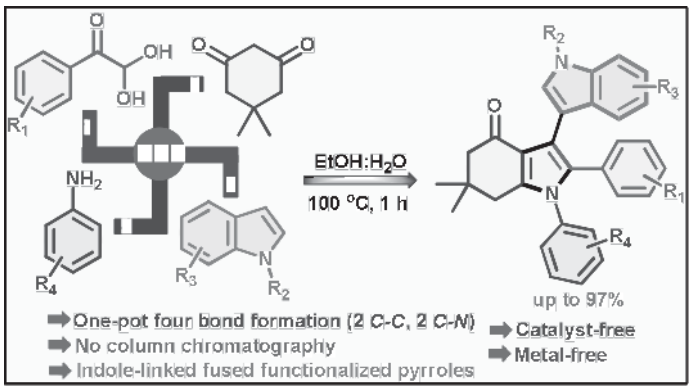
# Pot-, Atom-, and Step-Economic (PASE) Synthesis of Functionalized Fused Pyrroles

**RudranarayanSutar,**SwadhinSwaraj Acharya, and BibhutiBhusanParida*

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Heterocycles[1,2]are the unique molecular motifs broadly distributed in natural products, pharmaceuticals, and find applications in material chemistry as solar cells, metal ion sensors, and semiconductors. Consequently, the design and development of green synthetic methods has become an active area of research.[3] In the pursuit of green chemistry, the multicomponent reactions (MCRs) have been recognised as interesting tools which offer pot- and step-economic (PASE) approaches which are useful in the synthesis of bioactive heterocycles. Indoles[4] and pyrroles[5] are the celebrated molecules owing to their notablebioactivities. As a consequence, their synthesis is highly desirable. Herein, we present a PASE approach for the synthesis of functionalized fused pyrroles. The method operates under eco-friendly conditions and enables the rapid construction of molecular complexity in one-pot, while allowing gram-scale synthesis.




**Keywords:** Fused pyrrole, Indole, Multicomponent reactions, green chemistry

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# A Comprehensive Analysis of Lithium-Ion Battery Efficiency and Degradation

**Prajna Priyadarshini Rout, Guruprasad Dash**

## Abstract

Lithium-ion batteries (LIBs) have become essential energy-storage technologies for portable electronics, electric vehicles, and renewable-energy systems because of their high energy density, relatively low self-discharge, and long cycle life. However, progressive capacity loss, increasing internal resistance, and declining power capability during operation remain major challenges for their long-term performance and reliability. This study presents a comprehensive analysis of the factors governing LIB efficiency and degradation, with particular emphasis on electrochemical, thermal, and structural changes occurring during repeated charge–discharge cycles. Key degradation mechanisms include solid electrolyte interphase growth, lithium plating, loss of active electrode material, electrolyte decomposition, particle cracking, and impedance increase. Operating conditions such as temperature, charge/discharge rate, depth of discharge, state of charge, and upper cut-off voltage strongly influence the rate of degradation. Electrochemical techniques including galvanostatic charge–discharge analysis, cyclic voltammetry, and electrochemical impedance spectroscopy can be employed to evaluate capacity retention, coulombic efficiency, charge-transfer resistance, and changes in electrode kinetics. Thermal and structural characterization can further provide insights into degradation pathways. Understanding these mechanisms is important for optimizing battery operating conditions, improving electrode and electrolyte design, and extending battery service life. Such systematic analysis can contribute to the development of safer, more efficient, durable, and sustainable lithium-ion battery systems for next-generation energy-storage applications.

**Keywords:** Lithium-ion battery; Battery efficiency; Degradation mechanisms; Capacity retention; Coulombic efficiency; Solid electrolyte interphase; Energy storage.

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# What's Really on Your Plate? Exposing Food Adulteration from Farm to Fork

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**ABSTRACT**

Food adulteration is a clandestine and economically motivated practice that threatens public health, nutrition, and market integrity. From hazardous dyes such as Sudan Red and unscrupulous fillers like melamine to argemone oil in edible oils and urea or starch in dairy products, the range of adulterants demands rigorous scientific scrutiny. Chemical fingerprinting offers a forensic route to authentication by profiling characteristic molecular, elemental, and isotopic signatures. An analytical arsenal - including HPLC, GC-MS, LC-MS/MS, FTIR, Raman, and NMR - coupled with chemometric modelling enables sensitive detection and discrimination of adulterants even at trace levels. Comparison with authentic reference standards and established spectral databases strengthens regulatory and legal action. By illuminating the molecular evidence, chemists act as crucial guardians of the food supply, ensuring safety and authenticity from farm to fork. The development of rapid, reliable, and cost-effective fingerprinting strategies is therefore essential to keep pace with evolving adulteration practices and to protect consumer trust.

**Keywords**: Food Adulteration, dyes, argemone oil, spectroscopic analysis

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# From Molecular Interplay to Thermodynamic Insight: A Multimodal Ultrasonic, Spectroscopic and Statistical Investigation of Rifamycin–Arginine/Lysine Interactions

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**ABSTRACT :**

The present study proposes an integrated ultrasonic, spectroscopic and statistical investigation of the temperature-dependent molecular interactions of three important rifamycin-class antibiotics—Rifampin, Rifabutin and Rifapentine—with the biologically relevant amino acids L-arginine (Arg) and L-lysine (Lys) in aqueous media. The study is designed to elucidate the nature, strength and temperature dependence of drug–amino acid interactions, with particular emphasis on the molecular factors governing solute–solute association in aqueous environments. Such investigations are relevant to understanding drug–biomolecule interactions, molecular recognition, transport and the physicochemical behaviour of pharmaceutical compounds in biological systems.The experimental investigation will employ ultrasonic velocity, density and viscosity measurements over a suitable concentration and temperature range. These experimental parameters will be used to evaluate important acoustic and volumetric properties, including adiabatic compressibility, apparent molar volume, apparent molar compressibility, intermolecular free length, relaxation parameters and related derived quantities. The temperature dependence of these properties will provide information concerning changes in molecular packing, hydration, structural arrangement and the relative contribution of drug–amino acid and solute–solvent interactions. To complement the ultrasonic measurements, UV–Visible and FTIR spectroscopic techniques will be employed to identify possible changes in the electronic and vibrational environments of characteristic functional groups. Particular attention will be given to the structural features of the rifamycin derivatives and the amino, carboxylate and other potential interaction sites of arginine and lysine. Spectral shifts, intensity variations and changes in characteristic vibrational bands will be correlated with the acoustic and volumetric results to obtain a more comprehensive picture of the interaction mechanism.The thermodynamic aspects of the systems will be investigated through the temperature dependence of experimentally derived parameters, enabling estimation of relevant enthalpic and entropic contributions and assessment of the predominant forces involved, such as hydrogen bonding, electrostatic interactions, dipole–dipole interactions, hydrophobic association and hydration effects. Comparative analysis of Rifampin, Rifabutin and Rifapentine will help determine how structural modifications within the rifamycin family influence their interactions with Arg and Lys.A major feature of the study will be the application of statistical validation and multivariate analysis to establish correlations among ultrasonic, spectroscopic and thermodynamic parameters and to assess the reliability and significance of the observed trends. Statistical tools may also be used to distinguish temperature- and concentration-dependent effects and to identify parameters that most strongly characterize drug–amino acid association.Overall, the study aims to establish a multidimensional structure–interaction–temperature relationship for rifamycin antibiotics with arginine and lysine. The integrated findings are expected to provide deeper physicochemical insight into drug–amino acid interactions and contribute to a better understanding of the molecular behaviour of rifamycin-class drugs in aqueous and biologically relevant environments.

**Keywords :**Rifampin, Rifabutin, Rifapentine, Arginine, Lysine, Ultrasonic velocity,Adiabatic compressibility, Intermolecular free length, UV–Visible and FTIR analysis, Thermodynamics; Statistical validation, regression analysis and correlation coefficients.

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# APPLICATIONS OF POLYAROMATIC-METAL/METAL OXIDE COMPOSITES

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**Abstract:**

Polymers have always been considered as insulators of electricity. No one would have believed 40 years ago that polymers could conduct as good as metals. This is possible only by simple modification of ordinary organic conjugated polymers. They are called electrically conducting polymers or as synthetic metals. They combine the electrical properties of metals with the light weight, greater workability and resistance to corrosion of polymers. They are used in our day to day life with a wide range of products like applications in space, aeronautics, electronics etc.

Polypyrrole is one of the modern generations of polymeric materials which can be used as compact capacitors, antistatic coating, electromagnetic shielding and smart windows, capable to vary the amount of light to pass. It is mainly used due to its advantage as environmentally stable, easy to synthesise and high conductivity. Nanocomposites have attracted wide attention because of their potential to combine desirable properties of different nanoparticles to improve mechanical, optical, electronic, or magnetic properties. [1-6] There has been a growing interest in incorporating functional components, such as functional groups, polymers and nanoparticles, into the self-assembled nanostructures, however, success has been limited to two phase organic/inorganic hybrid materials, nanoparticles or polymer-based nanocomposites. [4,5,7,8] Polymer nanocomposites containing surface engineered metaloxide, or, silica, nanocomposites continuously offer new opportunities to enhance desired properties or, functionalities, such as optical transparency, ductility, flexibility or molecular mobility.[9-13]

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# Effect of Hydrophobic Tails and Hydrophilic Spacer Groupof Cationic Gemini Surfactants on Bovine Serum Albumin and Gelatin Proteins in Aqueous medium

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**Abstract**

This work demonstrates the refolding and unfolding mechanisms of bovine serum albumin (BSA, wt%) and gelatin (G, wt%) using cationic gemini surfactants with a diethyl ether (EE) spacer group (m−EE−m) and tails of varying lengths (m = 12, 14, and 16). Studies have been carried out by measuring UV−visible absorption, steady-state fluorescence and fluorescence anisotropy, and time-resolved fluorescence methods. The effects of hydrocarbon tail length and hydrophilic spacer on proteins were extensively studied. Micellisation, micropolarity, rigidity, and lifetime parameters showed that the longer the hydrophobic chain length, the greater the binding with BSA as well as Gelatin. Gemini surfactant 16-EE-16 has shown significant changes as compared to the other two surfactants having tail lengths of 12 and 14. Due to the hydrophilicity of the spacer group, the anisotropy decay becomes slower due to the formation of more compact micelles. The lifetime and anisotropy in gemini micelles are slower compared to those in their conventional counterpart. The lifetime decay is found to be triexponential, with lateral diffusion of the probe along the surface of the micelle as a slow component. Rotational motion of the micelle as a whole is a very slow process, and the motion becomes even slower with increasing size of the micelle. The structural advantages conferred by the presence of dual hydrophobic tails facilitate the formation of compact micellar assemblies, thereby reinforcing the applicability of gemini surfactants in pharmaceutical and materials science applications.

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# Esterification of native starch by isopropenyl acetateunder microwave activation and study of adsorption behaviour

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**Abstract**

Modification of native starch continues to be one among the versatile processes to tune the properties of starch. Among the various chemical pathways practised, esterification remains to be one of the most viable routes for modification [1]. In this work the modification of potato starch using i.e. isopropenyl acetate under microwave irradiation, detailed structural characterisation and studied its adsorption behaviour towards methylene blue reported.FE-SEM and HR-TEM analysis indicates change of smooth surface of native starch to a more rough and exposed structure. $^{1}$H NMR signals at δ value 1.86, 1.97 and 2.07 ppm in modified starch ascertained the insertion of isopropenyl acetate in starch framework. FT IR analysis indicates peaks at 1729 $cm^{-1}$ which establishes the bonding of isopropenyl acetate with starch.A mass fragmentation pattern obtained at m/z = 205 supported the replacement of hydroxyl by acetate group.The X-ray diffraction and thermo gravimetricstudies also supports the stiff and enhanced thermal stability of modified starch. The functionalization of native starch enhances marginally Tg and significantly Tc of modified starch [2]. As modified starch have open surface structure and polar carbonyl group attached to it. Hence adsorption capacity of esterified starch increases. The enhanced adsorption of methylene blue on isopropenyl acetate modified starch, ascertains the functionalization of native starch structure.

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# Advanced Electrode Materials for Next-Generation Lithium-Ion Batteries.

**Sumitra Baral[1], Guruprasad Dash**

## Abstract

The continuous growth of electric mobility, portable electronics, and renewable-energy systems has created a strong demand for lithium-ion batteries with higher energy density, longer cycle life, faster charging capability, and improved safety. Electrode materials play a central role in determining the electrochemical performance and practical limitations of lithium-ion batteries. This work highlights recent developments in advanced cathode and anode materials designed to improve lithium-ion storage and transport. High-nickel layered oxides, lithium-rich transition-metal oxides, silicon-based anodes, transition-metal oxides, phosphates, and carbon-based nanomaterials have attracted considerable attention because of their high theoretical capacities and tunable electrochemical properties. Nanostructuring, surface coating, elemental doping, defect engineering, and heterostructure formation can improve electrical conductivity, shorten lithium-ion diffusion pathways, and suppress structural degradation during repeated cycling. Electrochemical characterization through cyclic voltammetry, galvanostatic charge–discharge analysis, and electrochemical impedance spectroscopy provides valuable information regarding capacity, kinetics, rate capability, and interfacial resistance. Despite significant progress, challenges associated with electrode degradation, volume expansion, electrolyte compatibility, cost, and large-scale fabrication remain. Continued development of stable and sustainable electrode architectures is therefore essential for advancing high-performance lithium-ion battery technologies.

**Keywords:**Lithium-ion batteries; Advanced electrode materials; Cathode; Anode; Nano structuring; Energy density; Cycling stability;

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# Nanostructured Materials for Lithium-Ion Batteries

**KalpanaKishan, Guruprasad Dash**


## Abstract

Nanostructured materials have emerged as important components in the development of high-performance lithium-ion batteries because their nanoscale dimensions can provide large electroactive surface areas, short lithium-ion diffusion pathways, and enhanced electrode–electrolyte interactions. This study discusses the role of nanostructured materials, including graphene, carbon nanotubes, silicon nanoparticles, metal oxides, transition-metal sulfides, and nanocomposites, in improving the electrochemical performance of lithium-ion battery electrodes. Appropriate control of particle size, morphology, porosity, and surface chemistry can facilitate rapid ion and electron transport while accommodating structural changes during repeated lithiation and delithiation. In particular, carbon-based nanomaterials can improve the electrical conductivity of poorly conducting active materials, whereas nanostructured metal oxides and silicon-based materials can provide high theoretical capacity. Hybrid and hierarchical nanocomposite architectures further combine complementary properties to enhance rate capability and cycling stability. The electrochemical behavior of such materials can be assessed using cyclic voltammetry, galvanostatic charge–discharge measurements, electrochemical impedance spectroscopy, and long-term cycling tests. However, issues such as nanoparticle aggregation, high synthesis cost, surface instability, and scalability need to be addressed before widespread commercial implementation. Rational nanomaterial design and sustainable synthesis strategies can contribute significantly to the development of durable, high-energy lithium-ion batteries.


**Keywords:** Nanostructured materials; Lithium-ion batteries; Graphene; Nanocomposites; Metal oxides; Lithium-ion diffusion; Rate capability; Cycling stability.

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# Water-Soluble Pyridine-Functionalized Resorcin[4]arene Cavitands for Gold Nanoparticle Synthesis and Catalytic Applications

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**Abstract :**

Pyridine-functionalized resorcin[4]arene cavitands constitute a versatile class of supramolecular hosts that combine structural rigidity with tunable coordination and molecular recognition capabilities. Herein, we report a facile synthetic strategy for the preparation of two novel water-soluble resorcin[4]arene cavitands functionalized at the lower rim with 2-pyridyl and 4-pyridyl groups. Incorporation of pyridine moieties significantly enhances the aqueous solubility of the cavitand framework, thereby expanding its potential applications in water-based systems. The unusual water solubility imparted by the pyridine units, together with the presence of multiple hydroxyl groups, enables these cavitands to act as both reducing and stabilizing agents for the green synthesis of gold nanoparticles (AuNPs), eliminating the need for any external reducing agent. Using this approach, highly stable, non-aggregated spherical gold nanoparticles, Au@2-py-res and Au@4-py-res, were successfully synthesized. The formation, morphology, and stability of the nanoparticles were characterized by UV–Visible spectroscopy, transmission electron microscopy (TEM), and dynamic light scattering (DLS), revealing predominantly spherical particles with an average diameter of 22 ± 8 nm. Comparative studies revealed that the 4-pyridyl-functionalized cavitand produced a greater number of stable AuNPs than its 2-pyridyl analogue. This enhanced performance is attributed to the favorable spatial orientation of the 4-pyridyl groups, which facilitates more effective nanoparticle surface stabilization. Furthermore, the catalytic activity of the AuNPs stabilized by the 4-pyridyl cavitand (Au@4-py-res) was evaluated in the model reduction of 4-nitrophenol to 4-aminophenol using $NaBH_4$ as the reducing agent. The reaction followed pseudo-first-order kinetics with a rate constant of 0.125 $min^{-1}$ and achieved complete conversion within approximately 30 min. Overall, the water-soluble 4-pyridyl-functionalized resorcin[4]arene cavitand emerges as a multifunctional supramolecular platform that integrates host–guest recognition, nanoparticle generation, stabilization, and catalytic activity within a single molecular architecture, offering promising prospects for applications in catalysis, nanotechnology, and aqueous supramolecular chemistr.

**Keywords :** pyridine-functionalized resorcin[4]arene, Water-soluble cavitands, Gold nanoparticles(AuNPs) , catalysis, 4-Nitrophenol reduction

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# Sustainability-Driven Chemistry and Materials Science:Innovative Materials for Energy, Environmental Protection and Health

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**ABSTRACT**

The increasing demand for energy, environmental protection, and improved healthcare has created an urgent need for sustainable scientific and technological solutions. Chemistry and materials science play a central role in addressing these challenges by enabling the design, synthesis, characterization, and application of advanced materials with improved functionality and reduced environmental impact. This review discusses the emerging relationship between sustainable chemistry and materials science, with particular emphasis on innovation for energy, environmental remediation, and health applications. Advanced materials such as nanomaterials, metal oxides, perovskites, carbon-based materials, polymers, ceramics, composites, and two-dimensional materials are considered for applications in energy storage and conversion, photocatalysis, water purification, sensing, antimicrobial technologies, and biomedical systems. The integration of green synthesis, circular-economy principles, renewable resources, artificial intelligence, and materials-by-design approaches provides opportunities to reduce energy consumption, waste generation, and dependence on critical resources. Sustainable materials development requires simultaneous consideration of performance, resource availability, toxicity, recyclability, durability, and life-cycle environmental impact. Future innovation will increasingly depend on interdisciplinary collaboration between chemistry, materials science, engineering, environmental science, biology, and computational science. The development of multifunctional, low-cost, recyclable, and environmentally responsible materials can contribute significantly to a sustainable future while addressing global challenges in energy, environment, and health.

**Keywords:***Sustainability; Green chemistry; Materials science; Energy innovation; Environmental remediation; Healthcare materials; Nanomaterials; Renewable energy; Energy storage; Circular economy*.

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# Green Chemistry in Renewable Energy Technologies: Sustainable Materials and Energy Conversion.

**Barsharani Swain [1],Arpita Majhi[1],BijayalaxmiNayak[1], Guruprasad Dash**

**Abstract**

The increasing demand for clean energy and the environmental impacts associated with conventional energy technologies have intensified the need for sustainable approaches to energy production and conversion. Green chemistry provides a valuable framework for developing renewable-energy technologies by minimizing hazardous substances, reducing waste and energy consumption, and promoting the use of renewable and abundant resources. This abstract explores the application of green chemistry principles in the development of sustainable materials and processes for solar energy conversion, hydrogen production, fuel cells, batteries, supercapacitors, and biomass-derived energy systems. Particular attention is given to environmentally benign synthesis of nanomaterials and functional catalysts using renewable feedstocks, biomass-derived carbon materials, safer solvents, and energy-efficient processing methods. Such materials can facilitate important energy-conversion reactions, including water splitting, hydrogen evolution, oxygen reduction, carbon dioxide conversion, and solar-driven chemical transformations. Recent research also highlights the potential of biomass- and waste-derived carbon materials as sustainable electrodes and electrocatalysts for energy-storage and conversion applications. Integrating green chemistry with renewable-energy technologies can therefore contribute to reduced resource consumption, lower environmental impact, and development of circular energy systems. However, challenges remain in achieving scalable synthesis, long-term stability, high energy-conversion efficiency, economic feasibility, and comprehensive life-cycle sustainability. Continued integration of green synthesis, advanced materials chemistry, catalysis, and renewable-energy engineering can support the transition toward cleaner and more sustainable energy systems.

**Keywords:** Green chemistry; Renewable energy; Sustainable materials; Energy conversion; Green synthesis; Nanomaterials; Hydrogen production; Energy storage; Biomass; Circular economy.

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# Bio-accumulation and Risk Assessment of Heavy Metals in Fish Samples ofa Highly Polluted River-Estuarine Environment, India.

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**Abstract:**

Four species of fishes such as *Labeorohita, Labeocalabasu, Catlacatla* and *Ompakpabda*have been selected for the present study in Brahmani river basin, as all the four species are used by the local population as a common food source and are available in the study area. Various fish samples were collected from different stations of river Brahmani at the downstream of different environmentally important zones and were analyzed.

In the study the level of all the studied elements except Cr in all the four fish species are within the permissible limits of human consumption. However, the concentration of Cr in all the four zones of study area is in higher levels and exceptionally higher in Sukinda Mining Area probably due to Chromite mines waste water discharge from Sukinda Area and Jharkhand mines. The Cr Concentration in the present study in all four species is site specific corresponding with dissolved metals. Liver and kidney exhibited highest tendency to accumulate metals than muscle and gill. Highest levels of Cd, Pb, Cu and Zn in the liver of fishes like present study was also reported by Dural et al., (2007); Ploetz et al., (2007). The higher concentration of trace elements such as Pb and Cr in liver than other tissues might be due to strong coordination or affinity of metallothionein protein with these elements. Low level of Cu, Zn in fish muscles appears to be low levels of binding proteins in the muscles (Allen-Gill and Martynov, 1995).

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# Advanced Polymer Nanocomposites for Wastewater Treatment and Emerging Pollutant Removal

**Ritisnigdha Das, Lipsa mohanty, Rojali tripathy, Guruprasad Dash**

**Abstract**

The increasing discharge of industrial, pharmaceutical, agricultural, and domestic wastewater has resulted in the accumulation of diverse contaminants in aquatic environments, including dyes, antibiotics, pesticides, heavy metals, endocrine-disrupting compounds, and other emerging pollutants. Conventional wastewater treatment technologies often exhibit limitations in removing these persistent and trace-level contaminants. Advanced polymer nanocomposites (PNCs) have therefore attracted significant attention as multifunctional materials for efficient and sustainable water purification. Their unique combination of polymer matrices and nanoscale fillers provides enhanced surface area, tunable surface functionality, adsorption capacity, mechanical stability, and catalytic activity.Polymer nanocomposites incorporating metal oxides, carbon-based nanomaterials, graphene derivatives, carbon nanotubes, clays, and semiconductor nanoparticles can be designed for adsorption, membrane separation, photocatalytic degradation, and catalytic oxidation of wastewater contaminants. In particular, conducting and semiconductor-based polymer nanocomposites can facilitate visible-light-driven photocatalysis and promote the generation of reactive oxygen species for the degradation of recalcitrant organic pollutants. Nanocomposite membranes can additionally improve permeability, selectivity, antifouling properties, and contaminant rejection compared with conventional polymer membranes.

This presentation discusses recent advances in the synthesis, structural design, pollutant-removal mechanisms, and regeneration of polymer nanocomposites, with particular emphasis on emerging contaminants. The challenges associated with nanoparticle leaching, membrane fouling, long-term stability, scalability, toxicity, and environmental sustainability are also highlighted. Future development of recyclable, biodegradable, low-cost, and multifunctional polymer nanocomposites could contribute significantly to sustainable wastewater management and circular water-treatment technologies.

**Keywords:** Polymer nanocomposites; Wastewater treatment; Emerging pollutants; Adsorption; Photocatalysis; Nanocomposite membranes

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# Biodegradable Plastic Nanocomposites: Enhancing Mechanical Properties and Environmental Performance

**Saumitree khuntia, Pratyusha Priyadarshini Sahoo, Sasmita Sahoo Arpita Priyadarshini Barik, Guruprasad Dash**

**Abstract**

The growing accumulation of conventional petroleum-based plastics has intensified the need for sustainable materials that combine adequate performance with reduced environmental impact. Biodegradable plastic nanocomposites have emerged as promising alternatives by integrating biodegradable polymer matrices such as polylactic acid (PLA), polyhydroxyalkanoates (PHA), polybutylene succinate (PBS), and polybutylene adipate terephthalate (PBAT) with nanoscale reinforcing materials. Although biodegradable polymers offer environmental advantages, their practical applications can be restricted by relatively low mechanical strength, brittleness, poor barrier properties, and limited thermal stability. Incorporation of suitable nanofillers, including nanocellulose, nanoclays, silica, graphene-based materials, biochar, and selected metal or metal-oxide nanoparticles, can improve mechanical strength, stiffness, thermal stability, moisture and oxygen barrier performance, and functional properties.The nanoscale reinforcement can enhance polymer–filler interactions and create improved structure–property relationships while potentially reducing the quantity of polymer required for specific applications. These materials are particularly promising for sustainable food packaging, agricultural films, biomedical materials, and other disposable products. Recent research has also emphasized the importance of evaluating biodegradation, compostability, recyclability, nanoparticle migration, ecotoxicity, and life-cycle impacts rather than considering biodegradability alone as a measure of sustainability.This presentation discusses recent advances in the synthesis, characterization, and performance of biodegradable plastic nanocomposites, with particular emphasis on mechanical reinforcement, barrier properties, biodegradation, and environmental safety. The challenges of nanofiller dispersion, scalability, cost, end-of-life management, and potential micro/nanoplastic formation are also highlighted. The development of bio-based nanofillers and circular processing strategies could further improve the sustainability and practical applicability of these advanced materials.

**Keywords:** Biodegradable plastics; Polymer nanocomposites; Biopolymers; Nanofillers; PLA; Sustainable packaging; Biodegradation; Green materials; Circular economy; Environmental performance.

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# Agricultural Waste-Derived Nanoparticles: A Green Chemistry Approach to Sustainable Environmental Remediation

**Ranjit Pal, PradoshKumar Panda, Guruprasad Dash**

**Abstract**

The increasing generation of agricultural residues such as rice husk, straw, sugarcane bagasse, coconut shells, fruit peels, and other biomass wastes presents both an environmental challenge and an opportunity for developing sustainable value-added materials. Converting these abundant residues into nanoparticle-based materials represents an emerging green chemistry strategy that combines waste valorization with environmental remediation. Agricultural wastes contain cellulose, hemicellulose, lignin, silica, polyphenols, carbohydrates, and other bioactive components that can serve as precursors, reducing agents, stabilizing agents, or carbon sources for the synthesis of functional nanomaterials. Green processing approaches can reduce the use of hazardous chemicals, minimize energy consumption, and promote the development of low-cost and renewable remediation materials.Agricultural waste-derived nanoparticles and nanocomposites, including silica, metal oxides, carbon-based nanoparticles, and biogenic metal nanoparticles, exhibit high surface area, tunable surface chemistry, and enhanced adsorption or catalytic properties. These materials have demonstrated potential for the removal of dyes, antibiotics, pesticides, heavy metals, and other emerging contaminants from wastewater through adsorption, photocatalysis, catalytic oxidation, and advanced oxidation processes. In particular, biomass-derived carbon nanomaterials and metal-oxide nanocomposites can provide synergistic adsorption and photocatalytic degradation pathways. This approach also contributes to the circular economy by converting low-value agricultural residues into useful environmental remediation materials. However, challenges involving reproducibility, precursor variability, nanoparticle recovery, scalability, regeneration, potential nanoparticle release, and life-cycle assessment need further investigation. Overall, agricultural waste-derived nanomaterials offer a promising pathway toward integrating green chemistry, waste valorization, nanotechnology, and sustainable environmental remediation.

**Keywords:** Agricultural waste; Green chemistry; Waste valorization; Nanoparticles; Nanocomposites; Environmental remediation; Photocatalysis; Adsorption; Circular economy; Wastewater treatment.

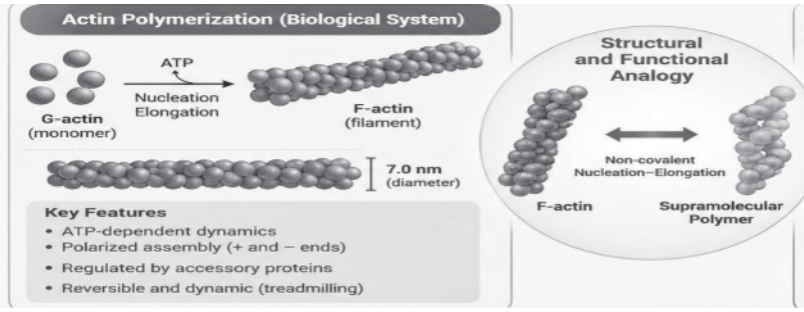
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# Supramolecular Polymers in Actin Science: Biomimetic Polymerization, Structural Dynamics, and Biomedical Applications.

UtkalKeshariSenapati [1], Guruprasad Dash




**Abstract**

Actin is a highly conserved cytoskeletal protein that undergoes dynamic and reversible assembly from globular actin (G-actin) monomers into filamentous actin (F-actin), forming a central component of the cellular cytoskeleton. The regulated polymerization and depolymerization of actin are essential for cell migration, cytokinesis, intracellular transport, and maintenance of cellular architecture. Supramolecular polymers, which are formed through reversible non-covalent interactions such as hydrogen bonding, hydrophobic interactions, –π stacking, electrostatic interactions, and host–guest recognition, provide valuable synthetic platforms for understanding and mimicking these dynamic biological assemblies. This study explores the conceptual relationship between actin filament formation and synthetic supramolecular polymerization, with particular emphasis on nucleation–elongation mechanisms, cooperative assembly, structural dynamics, and reversibility. Biomimetic systems based on peptide amphiphiles, benzene-1,3,5-tricarboxamides (BTAs), ureidopyrimidinone (UPy) motifs, and other self-assembling building blocks can generate high-aspect-ratio nanofibers and dynamic networks that reproduce selected structural and functional characteristics of cytoskeletal systems. Their assembly can be regulated by environmental stimuli such as pH, temperature, light, ionic strength, or chemical fuels. Such dynamic materials have potential applications in tissue engineering, drug delivery, biomimetic materials, regenerative medicine, and responsive hydrogels. Understanding the relationship between molecular recognition, supramolecular polymerization, and actin dynamics may provide new strategies for designing adaptive materials that reproduce selected features of living systems. The integration of supramolecular chemistry with actin biophysics therefore offers a promising framework for developing dynamic, self-healing, and biologically responsive materials.

**Keywords:** Supramolecular polymers; Actin; G-actin; F-actin; Biomimetic polymerization; Molecular recognition; Non-covalent interactions; Nucleation–elongation; Self-assembly; Biomedical applications.

Reference:1.Wang, H.; et al.From Supramolecular Polymers to Multi-Component Biomaterials. Chemical Society Reviews 2017, 46, 855–873.

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# Microplastics Pollution: A Global Challenge

Dr.MamataSahu

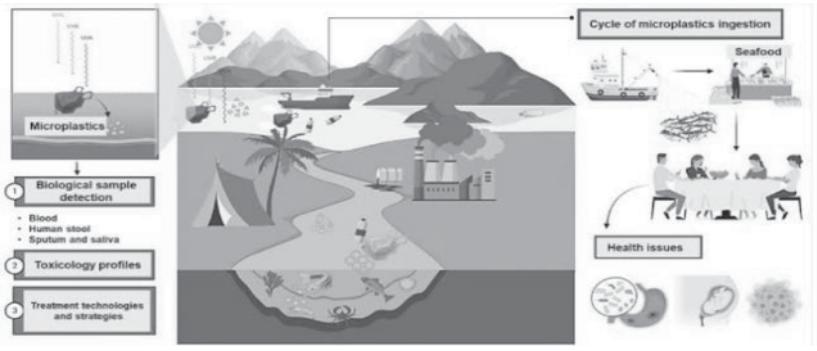
Choudwar College, Choudwar, Cuttack (Odisha)

Abstract:

Plastic pollution remains a global challenge and this alarming trend of rising plastic waste in India has severe consequences for the environment, wildlife, and human health. Microplastics (MP)s in water sources and food chains pose significant risks to human health, affecting the respiratory and reproductive systems and contributing to conditions like increased risk of cancer, male and female sterility, cardiovascular diseases, diabetes, and obesity.

Plasticswith a diameter of less than 5 mm which enter the human body through ingestion, inhalation or touch, but are not excreted, can be expected to accumulate in tissues of the human body. Additives to plastics are of major health concern include toxic metals, such as lead, cadmium, arsenic and chromium, bisphenol A (BPA). phthalates, brominated flame retardants (BFR) and endocrine- disrupting chemicals (EDCs). MPs being high specific surface area and hydrophobicity make them effective adsorbents of other pollutants. Consequently, ingestion of MPs by organisms can lead to significant harm to the ecosystem. This study offers anefficient cost-effective method for its removal.

Keywords: Microplastics, Chemical contaminants, Removal technique




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# Computational analysis of binding effectiveness for phytocompounds inhibition towards Sickle cell disease: DFT, Docking, AI/ML studies

**Subrat Kumar Pattanayak**

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**Abstract:**

Sickle cell disease is a hereditary hematological disorder primarily caused by a single amino acid substitution in the β-chain of hemoglobin. One major scientific issue is the creation of safer and more effective treatment compounds that target the molecular mechanisms of sickle hemoglobin. Selected phytochemicals form *Sorghum bicolor* screened against relevant molecular targets associated with sickle cell disease. Molecular docking employed to investigate ligand binding modes, binding affinities, hydrogen bonding, hydrophobic interactions, and key amino acid residues involved in molecular recognition. Then docked complexes subsequently be subjected to quantum chemical calculations using DFT to determine structural, electronic, and energetic properties, including HOMO-LUMO energies, energy gap, dipole moment, chemical hardness, and other reactivity descriptors. Furthermore, AI/ML models such as artificial neural networks (ANN), support vector machines (SVM), random forest (RF), and gradient-boosting approaches studied to establish relationships between molecular descriptors, docking scores, physicochemical properties, and predicted biological activity. These parameters correlated with docking-derived molecular interaction features to understand the structural basis of potential anti-sickling activity. The study could contribute to the development of computationally guided lead molecules and provide a framework for subsequent experimental validation in the discovery of novel anti-sickling agents in future.

**Key words:** *Sickle cell disease, Pharmacokinetics properties, Binding Energy.*

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# FRONTIERS IN CHEMISTRY AND CHEMICAL SCIENCES

**PRAVAT KUMAR BEHERA (M. Tech, Delhi University)**
**RESOURSE PERSON, DHSE, ODISHA**

**ABSTRACT**

In today's world, Chemistry and chemical sciences continue to evolve rapidly, fuelled by the growing demand for innovative solutions to global challenges such as disease management, renewable energy production, sustainable resource utilization, and environmental protection. The frontiers of chemistry now include multidisciplinary research that integrates biological, physical, engineering, and computational approaches along with artificial intelligence. Such convergence is accelerating scientific breakthroughs and flooring the way for transformative technologies with far-reaching societal impacts. Modern chemical research focuses on understanding matter at the molecular and atomic levels while translating this knowledge into practical applications that improve human life.

Some of the most exciting progress involves nanomaterials engineered for medicine, electronics, sensors, and environmental cleanup. Alongside this, green chemistry is transforming the field by championing eco-friendly processes, renewable materials, energy efficiency, and lower waste. Chemists are also driving the transition to clean energy through innovations in batteries, hydrogen fuel cells and solar cells (both silicon and polymer).

The integration of artificial intelligence and machine learning is revolutionising chemistry by speeding up how we design molecules, predict reactions, and discover new materials. Chemistry is also transforming medicine—fuelling new drugs, smart drug delivery systems, and advanced diagnostic tools which give researchers a clearer view of molecular processes than ever before.

When chemists, physicists, biologists, engineers, and data scientists join hands, breakthroughs happen much faster. chemistry continues to serve as a central science that connects various disciplines and transforms scientific knowledge into practical applications. The ever-expanding frontiers of chemistry and chemical sciences are shaping a future where groundbreaking innovations drive human progress, safeguard the planet, and ensure sustainable prosperity for generations to come.

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# Development and Electrochemical Performance of High-Energy Lithium-Ion Batteries

**Tanmayee Sahoo, Guruprasad Dash**

**Abstract**

The growing demand for high-performance energy-storage systems for electric vehicles, portable electronics, and renewable-energy integration has accelerated the development of high-energy lithium-ion batteries (LIBs). In the present study, emphasis is placed on the development of advanced lithium-ion battery materials and the evaluation of their electrochemical performance. The energy density, rate capability, cycling stability, and safety of LIBs are strongly influenced by the physicochemical properties and electrochemical behavior of their electrode materials. Advanced cathode materials, high-capacity anodes, conductive additives, and optimized electrolytes are therefore being investigated to improve charge-storage performance. Nanostructuring and surface engineering of electrode materials can provide shorter lithium-ion diffusion pathways, enhanced electrical conductivity, and improved electrode–electrolyte interactions. The electrochemical characteristics of the developed electrodes can be evaluated using cyclic voltammetry, galvanostatic charge–discharge measurements, electrochemical impedance spectroscopy, and cycling tests. Key parameters such as specific capacity, coulombic efficiency, energy density, power capability, charge-transfer resistance, and capacity retention are considered for performance assessment. Particular attention is also given to structural degradation, interfacial reactions, and volume changes that can limit long-term battery performance. The development of stable, high-capacity, and environmentally sustainable electrode materials, together with improved electrolyte and interface engineering, is expected to contribute to next-generation high-energy LIB technologies for efficient and reliable energy storage.

**Keywords:** Lithium-ion batteries; Energy storage; High-energy density; Electrode materials; Cycling stability.

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# Supramolecular Polymers in Microtubule Engineering: Molecular Design, Assembly and Biomedical Applications

**Aman Mishra, Guruprasad Dash**

**Abstract**

Supramolecular polymers are dynamic macromolecular systems formed through reversible, non-covalent interactions such as hydrogen bonding, π–π stacking, electrostatic interactions, hydrophobic forces, and host–guest recognition. Microtubules, which are cylindrical protein polymers composed primarily of α- and β-tubulin, are essential components of the cytoskeleton and play important roles in intracellular transport, cell division, and maintenance of cellular architecture. The integration of supramolecular polymer chemistry with microtubule systems provides an emerging strategy for controlling and mimicking dynamic biological architectures. Supramolecular polymers can be designed to interact with tubulin or microtubule surfaces through specific molecular recognition, enabling modulation of microtubule assembly, stabilization, destabilization, and organization. Such interactions can provide reversible control over microtubule dynamics while maintaining the dynamic nature characteristic of biological systems. Furthermore, supramolecular assemblies inspired by microtubular structures have potential applications in molecular transport, biomimetic materials, drug delivery, nanoreactors, and responsive nanodevices. Understanding the relationship between molecular recognition, supramolecular polymerization, and microtubule dynamics is therefore important for developing functional biohybrid materials. Continued advances in molecular design, microscopy, spectroscopy, and computational approaches are expected to facilitate the development of programmable supramolecular–microtubule systems for biomedical and nanotechnological applications.

**Keywords:** Supramolecular polymers; Microtubules; Tubulin; Molecular recognition; Non-covalent interactions; Biomimetic materials; Dynamic assembly; Nanotechnology.

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