

Virtual International Conference

**Title: Chemistry: Global Trends and
Future Directions-2024
(CGTFD-2024)**

Date: 05 - 07 August 2024



Organized by Department of Chemistry

**MADANAPALLE INSTITUTE OF TECHNOLOGY & SCIENCE
(UGC-AUTONOMOUS INSTITUTION)**

Madanapalle-517325, Annamaya Dist., Andhra Pradesh



**3-day Virtual International Conference
on
Chemistry: Global Trends and Future Directions
2024 (CGTFD-2024)**

Abstract Book

05-07, August 2024

**Organized by: Department of Chemistry
Madanapalle Institute of Technology & Science**

Foreword

The **Chemistry: Global Trends and Future Directions (CGTFD-2024)** has evolved into one of the foremost symposiums in chemistry. CGTFD-2024 has garnered significant interest, attracting over 152 registered participants from across the globe. The scientific program features 2 plenary talks, and 16 invited talks by experts in the field. Additionally, we are excited to welcome numerous young researchers from various countries to contribute to the discussions. The symposium includes 29 poster presentations by Ph.D. scholars, postdoctoral researchers and faculty members from nearly every region of the country.

We are particularly pleased to see a considerable number of M.Sc. students showing interest in participating in this symposium. CGTFD-2024 offers an excellent platform for engaging discussions, the exchange of ideas, and the opportunity to learn from peers and experts in related areas.

To facilitate easy access, we have organized the abstracts thematically. The Book of Abstracts provides a snapshot of current research trends in various areas and can be accessed electronically on the CGTFD-2024 website: <https://mits.ac.in/cgtfd2024/index.html>

We extend our heartfelt thanks to all participants and wish you fruitful and memorable discussions during this three-day virtual international conference. We also express our gratitude to our patrons and colleagues for their generous financial support.

Dr. Rashmi Roy (Convener)

Dr. Renjith Bhaskaran (HOD)
Dr. Amaladass P.
Dr. Lipika Rout
Dr. Sanoop P.
(Co-Convener)

**3-day Virtual International Conference
on
Chemistry: Global Trends and Future Directions (CGTFD-2024)**

Program Schedule

DAY 1 (05-08-2024)			
09.30-09.50 AM	Inauguration Conveners' speech: Dr. Rashmi Roy (Department of chemistry) HOD's speech: Dr. Renjith Bhaskaran (Department of chemistry) Conference Inauguration by Principal: Dr. C. Yuvaraj (Dept. of Mech. Engg.)		
Break			
Session 1 Chair: Dr. Arunbabu Dhamodaran			
10.00-10.45 AM	Plenary Lecture	Prof. C. P. Rao	SRM University, AP (Retired Professor from IIT Bombay)
Title of talk: <i>Supramolecular Conjugates of Calix[4]arenes: Multitude Application Domains</i>			
10.45-11.25 AM	Invited Speaker	Dr. Mohan Kumar K.	UNAM, Mexico
Title of talk: <i>Monitoring the charge transfer behaviour in Heterojunctions: Importance in artificial photosynthesis</i>			
Break			
Session 2 Chair: Dr. Boobalan Ramadoss			
11.40-12.20 PM	Invited Speaker	Dr. Arijit Kumar Dey	IISER Mohali
Title of talk: <i>A multidisciplinary approach toward solving the 'Global energy crisis'</i>			
12.20-1.00 PM	Invited Speaker	Dr. Raj Sharma	Aurigene Pharmaceutical services, Hyderabad
Title of talk: <i>Metal-catalyzed reactions - Industrial perspective</i>			
Break			
Session 3 Chair: Dr. C. V. Raju			
2.00-2.40 PM	Invited Speaker	Dr. Nitee Rathi	POSTECH, South Korea
Title of talk: <i>Catalytic Nanoprobes for Biofilm Eradication, Drug-Delivery, and Bioimaging</i>			
2.40-3.20 PM	Invited Speaker	Dr. Pavan Kancharla	IIT Guwahati
Title of talk: <i>Frustrated Brønsted Pair Catalysis for Glycoside Bond Formation</i>			
3.30-5.00 PM	Virtual Poster Session 1		
End of Day 1			

DAY 2 (06-08-2024)

Session 4 Chair: Dr. Rahul Pal

9.30-10.10 AM	Invited Speaker	Dr. Chayan Dutta	Georgia State University, USA
Title of talk: <i>Variable Non-Gaussian Transport of Nanoplastic on Supported Lipid Bilayers in Saline Conditions</i>			
10.10-10.50 AM	Invited Speaker	Dr. Thomas Stegmann	UNAM, Mexico
Title of talk: <i>Controlling the current flow in 2D materials</i>			
Break			
Session 5 Chair: Dr. V. Raju			
11.10-11.50 AM	Invited Speaker	Dr. Anandhu Mohan	Gachon University, South Korea
Title of talk: <i>Synthesis of Biomass-Derived Porous Carbon through Solid-State Activation for Reversible Iodine Capture</i>			
11.50-12.30 PM	Invited Speaker	Dr. Balaji Mohan	Madanapalle Institute of Technology & Science, AP, India
Title of talk: <i>Controlled Synthesis and Uniform Anchoring of Hollow Cu_xO Nanocubes on Carbon Nanofiber for Enhanced Se(S)-Se(S) Bond Activation</i>			
Break			
Session 6 Chair: Dr. Imran K.			
1.30-2.10 PM	Invited Speaker	Dr. Nadezda Prochukhan	Longitude Licensing Ltd. Dublin, Ireland
Title of talk: <i>Wood and wood-derived polymers for sustainable design of emerging applications</i>			
2.10-2.50 PM	Invited Speaker	Dr. Sumanta Sahoo	Yeungnam Univ. South Korea
Title of talk: <i>Impact of Metal Oxide and Sulfide-based Composites in Supercapacitor Technology</i>			
Break			
3.00-5.00 PM	Virtual Poster Session 2		
End of Day 2			

DAY 3 (07-08-2024)			
Session 7 Chair: Dr. R. Srinivasan			
9.15-10.00 AM	Plenary Lecture	Prof. Alexei V. Demchenko	Saint Louis University, USA
Title of talk: <i>From Stereocontrolled Glycosylation to Automated Chemical Synthesis of Glycans</i>			
10.00-10.40 AM	Invited Speaker	Dr. Satyajit Saha	ICT Mumbai, India
Title of talk: <i>Designing Multifunctional Aggregation Induced Emissive Luminogen by Precise Molecular Engineering</i>			
Break			
Session 8 Chair: Dr. Rajaram R.			
11.00-11.40 AM	Speaker	Dr. Manav Saxena	Jain University, Bangalore, India
Title of talk: <i>Fabrication of Large area Ultrathin Co/Ni(OH)₂ Flexible Nanosheets: Electrode Material for the Charge Storage and Water Splitting</i>			
11.40-12.20 PM	Speaker	Dr. Priyabrata Ghana	IIT Gandhinagar, India
Title of talk: <i>Transition Metal-Tetrel Multiple Bonds: Connecting Main Group Chemistry with Transition Metal Chemistry</i>			
Break			
Session 9 Chair: Dr. K. Ragavendran			
2.00-2.40 PM	Invited Speaker	Dr. Christopher Jeyakumar	The American College, Madurai, India
Title of talk: <i>Metal Catalysts for Nitrogen Activation & Reduction</i>			
2.40-3.20 PM	Invited Speaker	Dr. Bigyan Ranjan Jali	VSSUT, Orissa, India
Title of talk:			
Break			
3.20-4.30 PM	Virtual Poster Session 3		
4.30-5.00 PM	Valedictory function		



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Co-convener

Dr. Lipeeka Rout

Assistant Professor



Co-convener

Dr. Sanoop P

Assistant Professor

CGTFD-24 Poster Presentation Schedule		
Day-1 (05-08-2024) Poster's list (Time: 03.30 - 05.00 PM IST)		
Poster No.	Name of the Participant	Institute Name
P1	Subrata Patra	University of Bern, Switzerland
P2	Arti Saroj	IIT(BHU) Varanasi
P3	Monisha Arumugama	SRM Institute of Science and Technology, Kattankulathur
P4	Sarita	Govt. Meera Girls College, Udaipur, Rajasthan
P5	P. Suresh	GITAM (Deemed to be University), Visakhapatnam, Andhra Pradesh
P6	Sayali Patil	Jain Global Campus, Bangalore
P7	R. Ganesamoorthy	Vinayaka Mission's Kirupananda Variyar Arts and Science College,
P8	Milind Digamber Kulkarni	NIMS, Rajasthan
Day-2 (06-08-2024) Poster's list (Time: 03.00 - 05.00 PM IST)		
P9	Chetana Deoghare	Indus University, <i>Ahmedabad</i> , Gujarat
P10	Andriambahiny Ranto Ny Aina	Parul University, Vadodara, India
P11	Nidhi Pathak	Central University of Gujarat, Gandhinagar
P12	K. Balakrishna	GITAM (Deemed to be University), Visakhapatnam, Andhra Pradesh
P13	Aditya D. S.	Jain Global Campus, Jain University, Bangalore
P14	Shanmuga Priya S	Vellore Institute of Technology, Vellore
P15	Kabir Hussain	Vellore Institute of Technology, Vellore
P16	Rikitha S Fernandes	Birla Institute of Technology and Science Pilani, Hyderabad Campus
P17	Kamatham Narayanaswamy	SRM University – AP
P18	Naveena S. Veeranaiaiah	Central University of Karnataka
P19	K. Premlatha	Annai Violet Arts and science College, Chennai
P20	Sneha Mondal	CNMS, Jain University
Day-3 (07-08-2024) Poster's list (Time: 03.30 AM - 5.00 PM IST)		
P21	Pratikkumar Lakhani	The Maharaja Sayajirao University of Baroda
P22	Rahul Ajit Durgannavar	Jain (Deemed-to-be University), Jain Global Campus, Bangalore
P23	Ragavi. S. P.	Vellore Institute of Technology, Vellore
P24	Shalini Dyagalaa	Birla Institute of Technology & Science (BITS) Pilani
P25	Manu M. Joseph	CHRIST University, Bangalore
P26	Thangaraja Gnanadurai Vimalraj	Periyar University, Salem
P27	Mausami	Mahila Mahavidyalaya, Banaras Hindu University, Varanasi
P28	Sammitha D. Hebbar	National Institute of Technology Karnataka (NITK), Surathkal
P29	Wiqar Uddin	Hazara University Mansehra Pakistan

From Stereocontrolled Glycosylation to Automated Chemical Synthesis of Glycans

Prof. Alexei V. Demchenko
Department of Chemistry, Saint Louis University, USA.

From the building blocks of nature to disease-battling pharmaceuticals, carbohydrates have had a profound impact on evolution, society, the economy, and human health. Numerous applications of these essential biomolecules in many areas of science and technology exist, most of which can be found at the forefront of therapeutic agent and diagnostic platform development. Although carbohydrates are desirable for the pharmaceutical and biomedical communities, these molecules are very challenging targets for chemists because of the need for functionalization, protecting and leaving group manipulations, controlling anomeric stereoselectivity, separation, and analysis. The development of practical methods for the synthesis of building blocks, chemical glycosylation, and glycan assembly represents demanding areas of research.



At the core of this presentation is the development of new methods, strategies, and technologies for the chemical synthesis of glycans. These tools will be discussed in light of recent results related to the development of new glycosylation reactions, methods for controlling stereoselectivity, and HPLC-based automated synthesis. The effectiveness of the methods developed will be illustrated by the synthesis of glycopharmaceuticals. This work has been generously supported by the National Institutes of Health and the National Science Foundation.

Supramolecular Conjugates of Calix[4]arenes: Multitude Application Domains

Chebrolu Pulla Rao

Department of Chemistry, SRM University AP, Neerukonda (P.O.), Guntur (dist)-522 240, Andhra Pradesh, India. (E-mail: cp.rao@srmmap.edu.in)

Activity concerned with the synthesis of the conjugates of calix[n]arenes *via* organic derivatization affecting the lower rim or the upper rim or both has become routine among chemists who work on this class of supramolecules. The current literature is abundant with the synthetic designs. When the advantages of these two aspects are taken into consideration, it is not impossible to develop and synthesize the conjugates of calixarenes suitable to perform specific function. Recent developments of these by anchoring on to the solid surfaces have elevated their utility in a variety of fields. Thus, there lies a tremendous potential for properly designed and carefully tailored conjugates of calix[n]arenes to serve as materials for multitude applications and thus the influence of calixarenes has gone much beyond sensing. During the past one and half decades, our group entered into the arena where the conjugates of calixarenes are appropriately designed, synthesized and demonstrated for their cell targeting, anticancer activity, drug delivery, gene transfer, catalysis and in water purification.¹⁻¹¹ Our efforts go much beyond in comparing our systems with those reported in the literature ones as a proof for their versatility.¹²⁻¹⁶ Several of these will be a part of this lecture.



I acknowledge DST/SERB, CSIR, DAE-BRNS for financial support, IIT Bombay for infrastructure and Chair Professorship in the past, and IIT Tirupati for the MHRD professorship and DST for JC Bose National Fellowship, and all my co-workers and collaborators for contributing to this research. I thank SRM University AP for my current position as senior professor.

- (1) *ACS App. Mat. & Interfaces*, **2017**, 9, 5109-5117 & **2016**, 8, 3135-3142 & **2015**, 7, 11555-11566.
- (2) *ACS Sustainable Chemistry & Engg.* **2017**, 6, 8882-8890.
- (3) *Anal. Chem.*, **2015**, 87, 9344-9351 & 4988-4995.
- (4) *ACS Omega* **2020**, 5, 21288-21299 & 25747-25756; **2019**, 4, 4908-4917, 5731-5740 & 7723-7733; **2018**, 3, 229-239 & 16989-16999.
- (5) *J. Org. Chem.* **2018**, 83, 11850-11859.
- (6) *Chem. Eur. J.*, **2016**, 22, 8980-8989 & 8903-8914 & **2015**, 21, 13364-13374.
- (7) *Chemistry Select*, **2018**, 3, 1248-1256.
- (8) *Dalton Trans*, **2015**, 44, 1130-1141.
- (9) *J. Org. Chem.* **2018**, 83, 11850-11859.
- (10) *Inorg. Chim. Acta* **2018**, 483, 337-342.
- (11) *Supramol. Chem.* **2018**, 30, 619-626.
- (12) *J. Chem. Sci.* **2021**, 133, 92
- (13) *Chem. Commun.*, **2022**, 58, 6044-6063
- (14) *J. Mat. Chem. B* **2021**, 9, 3523-3532
- (15) *Coord. Chem. Revs.* **2023**, 493, 215256
- (16) *Langmuir* **2024**, 40, 4579 -4591.

Multidisciplinary Approach Toward Solving the ‘Global Energy Crisis

Dr. Arijit Kumar De
Department of Chemical Sciences, IISER Mohali, India.

A global energy crisis is rapidly growing and consumption of limited energy resources (e.g., fossil fuels) demands the development of new sustainable energy resources. Sunlight is one of the potential natural energy sources. The remarkable efficiency of sunlight harvesting in photosynthesis has motivated researchers to study energy and charge transfer dynamics in photosynthetic pigment-protein complexes as well as rationally designed artificial photosynthetic analogues to capture, store and utilize sunlight most efficiently and inexpensively.



While our group has been exploring, through a combination of experiments and theories, a multitude of multidisciplinary problems spanning chemistry, biophysics, and condensed matter physics, keeping in mind of this grand challenge of global energy crisis, the main focus has been to investigate energy and charge (electron/hole or proton) transfer dynamics, covering a wide range of timescales (few tens of femtoseconds to few tens of nanoseconds), within systems of varying complexities (namely, organic chromophores and their aggregates/multichromophoric systems, transition metal complexes, halide perovskites and fluorescent proteins) and the effect of the local environment (for example, solvation and nanoscale confinement) on it. To study these problems, we developed a couple of cutting-edge spectroscopic techniques.

In this talk, I will discuss how we can think about solving the challenge of the ever-increasing demand of energy of the world through a multifaceted approach combining the expertise of different disciplines of science and technology.

Metal-catalyzed Reactions - Industrial Perspective

Dr. Raj Sharma

Director - Business development lead for Europe Business



In pharmaceutical space, transition metal catalysis has become foundational reaction for drug discovery, development, and manufacturing. Starting from numerous cross-coupling methodologies that facilitate simple construction of C–C and C–X bonds, to asymmetric hydrogenations that almost trivialize the construction of numerous primary and secondary stereocenters, transition metal catalyzed reactions has become widely utilized across the chemical community ranging from medicinal chemistry all the way to commercial manufacturing in pharmaceutical industry. Remarkably, the Suzuki–Miyaura and Buchwald–Hartwig reactions are now among the top five reactions performed by medicinal chemists today, which facilitates the design of modern pharmaceuticals. Interestingly, the predictable nature and detailed understanding of the mechanism of these transformations, along with the broad commercial availability of diverse coupling partners and catalysts, make these reactions appealing within the drug discovery space. For the process chemist, it is often difficult to envision constructing molecules and organic scaffolds without employing these venerable reactions. While pharmaceutical industry is driven by sustainability and cost, fortunately, the goals of green chemistry and process chemistry are very much parallel, and transition metal catalysis intersects with these goals directly. Also, catalysis is number 9 on the list of the 12 principles of green chemistry, set forth by Paul Anastas and John Warner, but it would be incomplete understanding to think that all catalysis is green, and this is especially true for transition metal catalysis. In the talk, the discussion would be focused on how various chemists utilize and envision transition-metal catalyzed reactions during various stages of drug discovery and development.

Variable Non-Gaussian Transport of Nanoplastic on Supported Lipid Bilayers in Saline Conditions

Chayan Dutta¹

¹*Department of Chemistry, Georgia State University, Atlanta, GA, USA 30303*

Plastic nanoparticles (PNPs) have recently emerged as a significant concern due to their potential adverse impacts on biosystems. Small size and high surface-to-volume ratio facilitate nanoparticle interactions with lipid membranes, leading to structural modifications and long-term accumulation within membranes, ultimately resulting in functional changes. However, comprehending the effects of PNPs on biosystems is challenged by their physicochemical heterogeneity. Thus, nanoscale single-particle measurements are necessary to elucidate the impact of particle variability and their fate by analyzing PNPs' transport properties on biomembranes. We investigated PNP transport on biomimetic membrane surfaces under different ionic strength conditions, using single particle tracking (SPT) analysis. We employed a home-built total internal reflection fluorescence (TIRF) microscope to probe particle transport on model lipid surfaces. We compared the transport of fluorescently labeled carboxy-functionalized polystyrene (PS) particles on a supported lipid bilayer made of 1-palmitoyl-2-oleoyl-sn-glycerol-3-phosphocholine (POPC) under various conditions to identify the salt effects on the PS transport process. Our results show an ionic strength-dependent transport of PS nanoplastics and increased confinement at high salt environments. Additionally, we tested environmentally relevant PNP samples to understand the effects of particle heterogeneity. We correlated changes in diffusion properties and surface residence times of PNPs to alterations in the electrostatic interactions and hydrophobic effects between the PS and the POPC membrane surface. These preliminary investigations represent a foundational step towards understanding the fundamental physicochemistry of PNPs, shedding light on nanoscale interactions at the single-particle level, and will allow us to investigate the biophysical implications of these interactions.



Catalytic Nanoprobes for Biofilm Eradication, Drug-Delivery, and Bioimaging

Dr. Nitee Rathi

Department of Chemistry, POSTECH, South Korea.



Designing and synthesizing catalytic nanostructures and fine-controlling their properties can be highly useful for biomedical and healthcare applications. We synthesized mixed-FeCo-oxide-based surface-textured nanostructures (*MTex*) as highly efficient magneto-catalytic platforms.^[1] *MTex* can produce defensive reactive oxygen species (ROS) over a broad pH range and can effectively diffuse into the biofilm and kill the embedded bacteria. The unique surface topography and bimetallic composition with oxygen vacancies of *MTex* are the key features for high performance. *MTex* proved to be highly advantageous over the existing antimicrobials. In another example, we synthesized Au/Pt-based Janus nanostructures, like “egg-in-nest” morphology (*Au/Pt-ENs*) demonstrating as catalytic glucose-fueled autonomously motile drug-delivery platform.^[2] We implemented a new ‘dynamic-casting approach’ using silica yolk-shell cast providing the anisotropically confined concave hollow nanospace to grow curved Pt-dendritic porous networks. *Au/Pt-ENs* showed enhanced motion as a result of dual enzyme-relay-like catalytic cascade at Au-Pt interfacial site oxidizing glucose in physiological biomedica, and in turn showing molecular-laden transport to living cells. As a key *catalytic-motile* feature, high diffusiophoresis in cell culture media increased the nanomotor-membrane interaction events and in turn facilitated the cell internalization while delivering the drug-molecule cargo. Ascertaining the locations of nanostructures inside cell by their innate bioimaging modality would be highly advantageous. In this regard, silica-derived silicon (Si) is useful semiconductor material due to its high biocompatibility, stability and innate photoluminescence. We synthesized hydrophilic Si-nanoshells encapsulated with catalytic PdNCs in a *rattle-like* configuration.^[3] Due to small size and hydrophilicity, these nanoprobes were easily endocytosed inside mammalian cells, demonstrating high biocompatibility and photostable Si characteristic PL-based live cell imaging. Intracellular Si-nanoprobes demonstrated excellent catalysis to synthesize bioimaging molecules as the result of light-induced heterogeneous [Pd]-catalyzed C–C cross-coupling reaction. By the development of new nanoscale chemistries, highly functional nanomaterials can be designed and synthesized. I will discuss key synthetic strategies and their applications, which our group has recently introduced.

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[1] *Nano Lett.* **2021**, *21*, 279–287

[2] *Angew. Chem. Int. Ed.* **2021**, *60*, 17579–17586

[3] *Small* **2023**, *19*, 2301190

[3] *J. Am. Chem. Soc.* **2018**, *140*, 15176–15180

Title: Frustrated Bronsted Pair Catalysis for Glycoside Bond Formation

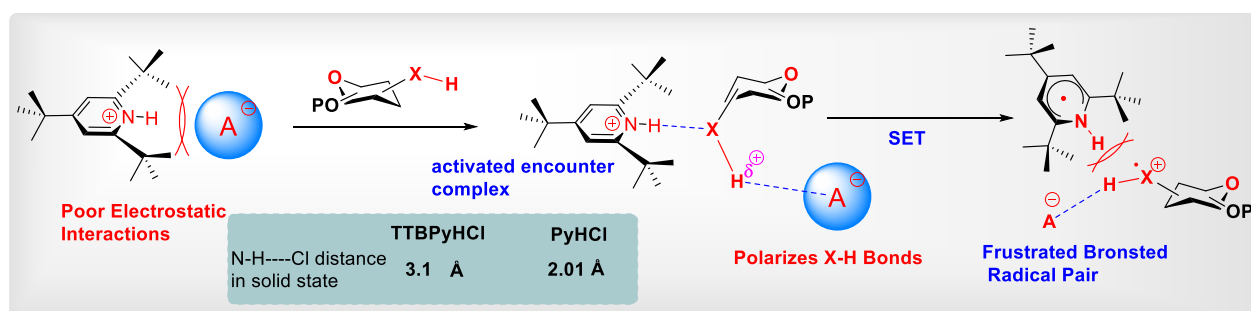
Dr. Pavan K. Kancharla

Department of Chemistry, Indian Institute of Technology Guwahati

Organocatalysis has emerged as a significant tool for organic synthesis over past two decades. Enormous progress has been made in utilizing the small molecule organocatalysis to control organic reactions' enantioselectivity and diastereoselectivity. Glycosylation is arguably the most significant reaction in carbohydrate chemistry and controlling the anomeric selectivity in glycosylation reactions is of prime importance. Our laboratory is focused on developing new organocatalytic methods for the construction of various glycosidic linkages and controlling the anomeric selectivities. The focus of the talk will be mainly on one of the unique concepts developed in our laboratory, “Frustrated Bronsted-Pair Catalysis” and including some of the other aspects of glycoside bond formation



the



References and Notes:

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2. Addanki, R. B.; Halder, S. H.; Kancharla, P. K. *Org. Lett.* **2022**, 24, 1465-1470.
3. Mukherji, A.; Addanki, R. B.; Halder, S. H.; Kancharla, P. K. *J. Org. Chem.* **2021**, 86, 17226.
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5. Ghosh, T.; Mukherji, A.; Kancharla, P. K. *Org. Lett.* **2019**, 21, 3490–3495.

Monitoring the charge transfer behaviour in Heterojunctions: Importance in artificial photosynthesis

Dr. Mohan Kumar Kesarla

Investigador Titular A de TC

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Universidad Nacional Autónoma de México, Av. Universidad s/n, Cuernavaca, Morelos, C.P. 62210,
México*

This talk focuses on the importance of heterojunction photocatalysts and their charge transfer behavior. Some basic concepts that must be considered during its use in energy and environmental catalysis will be covered, which includes basics of water splitting with semiconductor-photocatalysts, the problems associated with single semiconductor photocatalysts and how heterojunctions can overcome these problems and finally designing the heterojunctions and their characterization using various techniques to understand the behavior of charge transfer. In addition, recent work on energy and environmental catalysis through heterojunctions that we developed in the materials science group will be briefly presented.



Impact of Metal Oxide and Sulfide-based Composites in Supercapacitor Technology

Dr. Sumanta Sahoo
Assistant Professor
School of Chemical Engineering
Yeungnam University



Energy has become a vital component of the modern world. The crisis of such a crucial component has become a global issue today. To overcome this, modern science and technology have been significantly focused on exploring alternating energy resources. Supercapacitor (SC) is one such electrochemical energy storage device that expressively advances the modern automobile industry. In this talk, the basics of SC technology will be discussed in detail. Special attention will be paid to exploring fruitful strategies for improving the electrochemical performance of SC electrodes based on the composites of metal oxide/mixed metal oxides and metal sulfides/mixed metal sulfides. Furthermore, the efficient ways of enhancing the device's performance will also be explored in this talk. Various synthetic strategies of the metal oxides and sulfides and their composites with advanced 2D materials like MXene, graphene, etc. will also be focused.

Synthesis of Biomass-Derived Porous Carbon through Solid-State Activation for Reversible Iodine Capture

Dr. Ananhu Mohan

Department of Nano Science and Technology Convergence, Gachon University, South Korea.

The search for adsorbent materials capable of extracting and storing radioactive iodine derived from nuclear power plants has intensified owing to the growing nuclear waste concerns. Herein, we introduce a novel method, which is simple and effective, to synthesize biomass-derived porous carbon from an easily available biomass, *Opuntia humifusa*, via simple solid-state activation with zinc chloride. The resulting porous carbon exhibits a large specific surface area, with up to 1869 m²/g of micropores. The textural properties of activated carbons can be easily modified by adjusting the amount of zinc chloride and activation temperature. The optimal conditions were found to be a ZnCl₂ to biomass ratio of 5 and a carbonization temperature of 500 °C. The obtained porous carbons can function as multifunctional solid sorbents for radioactive iodine because of their high porosity and advantageous hierarchical porous structure. Specifically, the obtained activated carbon exhibited high iodine affinity with an absorption of 408 wt%. Considering its global abundance and recyclability, *Opuntia humifusa* can be used as a new biomass source for the efficient production of highly effective porous carbon materials with potential applications in environmental restoration. Furthermore, the straightforward single-step synthesis method described in this study offers a technique for producing several unique activated mesoporous carbons from various biomasses.

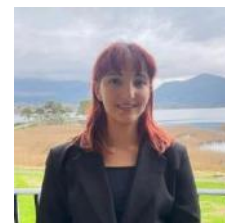


Keywords: *Biomass-derived carbon, Opuntia humifusa, single-step solid-state activation, reversible capture of iodine.*

Wood and wood-derived polymers for sustainable design of emerging applications.

*Dr. Nadezda Prochukhan
Member of Technical Staff, Longitude Licensing Ltd.
Dublin, Ireland.*

Modern and emerging technologies rely on fast development and research and often disregard the environmental cost. However, the global ecological crisis has raised awareness about the importance of sustainability and circularity from the onset of the manufacturing process. It is crucial to employ methods with the least hazardous approach possible using green and biodegradable resources.



Wood is an abundant biomaterial which is often used in construction as well as for energy generation. However, it has interesting properties such as strength and durability and inherent biodegradability. In our research, we utilise scrap wood material such as twigs, bark and logs from various species such as pine, oak, beech as well as mixed chips to design new materials such as filters and transparent wood as a cost- and eco-effective substitute for glass. Wood can also be mechanically processed such as with application of heat, stress, pressure and chemical treated (bleaching in hot hydroxide solution) to yield ultra-strong wood. Thus, the material which is treated as waste by sawmills can be upcycled to various ecologically relevant applications.

Wood also contains the two most abundant biopolymers namely cellulose and lignin. Cellulose is used in the paper making industry; however, lignin is often treated as a by-product. Only recently has it gained visibility as a material that can be used in energy storage or fuel applications. In our research lignin was used to produce membranes for the first time without additives and the resultant structure was templated onto silicon to yield black silicon, a light absorber useful for solar cell technology. We have also demonstrated the generation of cellulose membranes by the same principle.

Thus, we demonstrate the use of wood as well as its constituent polymers (lignin and cellulose) for various environmentally important applications in a sustainable manner.

Controlling the current flow in 2D materials

Dr. Thomas Stegmann

Department of Physics, National Autonomous University of Mexico, Mexico

In this talk, we will address some strategies to control the current flow in 2D materials. In the first part of this talk, we demonstrate that the current flow in graphene can be guided on atomically thin current pathways by the engineering of Kekule-O distortions. A grain boundary in these distortions separates the system into topologically distinct regions and induces a ballistic domain-wall state. The state is independent of the orientation of the grain boundary with respect to the graphene sublattice and permits guiding the current on arbitrary paths. As the state is gapped, the current flow can be switched by electrostatic gates. An atomic model supported by DFT calculations demonstrates that the system can be realized by decorating graphene with Ti atoms. [1] In the second part of this talk, we propose a nanoelectronic device made of twisted bilayer graphene (TBLG) to steer the direction of the current flow. The ballistic electron current, injected at one edge of the bottom layer, can be guided predominantly to one of the lateral edges of the top layer. The current is steered to the opposite lateral edge, if either the twist angle is reversed or the electrons are injected in the valence band instead of the conduction band, making it possible to control the current flow by electric gates. [2]



[1] S. Galván y García, Y. Betancur-Ocampo, F. Sánchez-Ochoa, T. Stegmann: *Nano Letters* 24: 2322 (2024)

[2] J. A. Sánchez-Sánchez, M. Navarro-Espino, Y. Betancur-Ocampo, J.E. Eduardo Barrios-Vargas, T. Stegmann: *J. Phys. Mater.* 5: 024003 (2022).

Designing Multifunctional Aggregation Induced Emissive Luminogen by Precise Molecular Engineering

Dr. Satyajit Saha
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The application of fluorescent materials in several areas has incited extensive research activities on fluorophores during the last two decades.¹ Despite the abundance of several types of fluorescent materials like organic dyes, organic-metal complexes, and quantum dots, there is a continuous pursuit of developing fluorescent materials that do not suffer from emission quenching at higher concentrations. The deleterious emission quenching phenomenon known as aggregation-caused quenching (ACQ) greatly restricted the widespread use of fluorophores in concentrated form. Often the diluted fluorophores or dispersed fluorophores at low concentrations result in severe photobleaching leading to a low target-to-background ratio (TBR), with drastically diminished sensitivity, thereby restricting their applicability. The ground-breaking discovery of the AIE phenomenon by Tang and co-workers in 2001 mitigated the ACQ problem and amplified the global research on small molecule AIEgens for diverse applications like metal sensing, bioimaging, organic light-emitting diodes, nanomaterials, etc.² Although challenging, it is of great significance, to regulate the molecular properties of AIEgens precisely by rational molecular designing. We are going to discuss how in our research group we have taken up the molecular engineering concept to rationally design multi-functional aggregation induced emissive luminogens.³

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Fabrication of Large area Ultrathin Co/Ni(OH)₂ Flexible Nanosheets: Electrode Material for the Charge Storage and Water Splitting

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Bifunctional electrode materials are highly desirable for meeting increasing global energy demands and mitigating environmental impact. However, improving the atom-efficiency, scalability, and cost-effectiveness of storage systems, as well as optimizing conversion processes to enhance overall energy utilization and sustainability, remains a significant challenge for their application. Herein, we devised an optimized, facile, economic, and scalable synthesis of large area (cm²), ultrathin (<5 nm) electroactive nanosheet of Co(OH)₂ and β-Ni(OH)₂, which acted as bifunctional electrode material for charge storage and oxygen evolution reaction (OER). These electrodes show better activity as compared to their bulk counterpart.

Further the rapid miniaturization of portable and wearable electronics and next-generation electronics rely on miniaturized energy storage devices such as “micro-supercapacitor” (MSC) that provide flexibility and portability. Volumetric capacitance is the most significant metric for miniaturized capacitive energy storage units due to the limitations in device volume and active surface area. Herein, we have used a flat 3.5 nm 2D ultrathin Co(OH)₂ nanosheet as an electrode material for the flexible, solid-state micro-supercapacitor on micropatterned laser-scribed graphene (LSG) and PVA/KOH gel electrolyte. The present research work opens a new avenue for the simple and scalable manufacture of ultrathin film-based electrode material research.

1. [Facile and scalable fabrication of flexible micro-supercapacitor with high volumetric performance based on ultrathin Co\(OH\)₂ nanosheets](#), *J. Mater. Chem. A*, 2024, Advance Article. DOI: 10.1039/D4TA02916J
2. [Large-area ultrathin 2D Co\(OH\)₂ nanosheets: a bifunctional electrode material for supercapacitor and water oxidation](#), *Mater. Today Energy*, 2024, 44, 101608
3. [Ultrathin, large area β-Ni\(OH\)₂ crystalline nanosheet as bifunctional electrode material for charge storage and oxygen evolution reaction](#), *J. Colloid Interface Sci.*, 2024, 674, 587.

Transition Metal-Tetrel Multiple Bonds: Connecting Main Group Chemistry with Transition Metal Chemistry

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The chemistry of compounds featuring triple bonds of the heavier Group-14 elements Si–Pb with transition metals is a very challenging research area, which combines modern molecular main-group elements with transition-metal chemistry and is of fundamental importance for the understanding of chemical bonding. During the last 30 years, the research in this area has witnessed considerable progress in isolating a series of closed-shell heavier tetrylidyne complexes.^[1] However, despite numerous attempts, open-shell tetrylidyne complexes with tetrel center unpaired electron and heavier group 14 element congeners of metallacarbonyl complexes remained inaccessible. In the first part of this talk, the story of the first open-shell heavier tetrylidyne complexes featuring a tetrel-center unpaired electron (**I**), and the unprecedented metallasilylidyne (**II**) containing a multiply bonded, linear-coordinated silicon atom embedded between two metal centers will be presented.^[2,3]

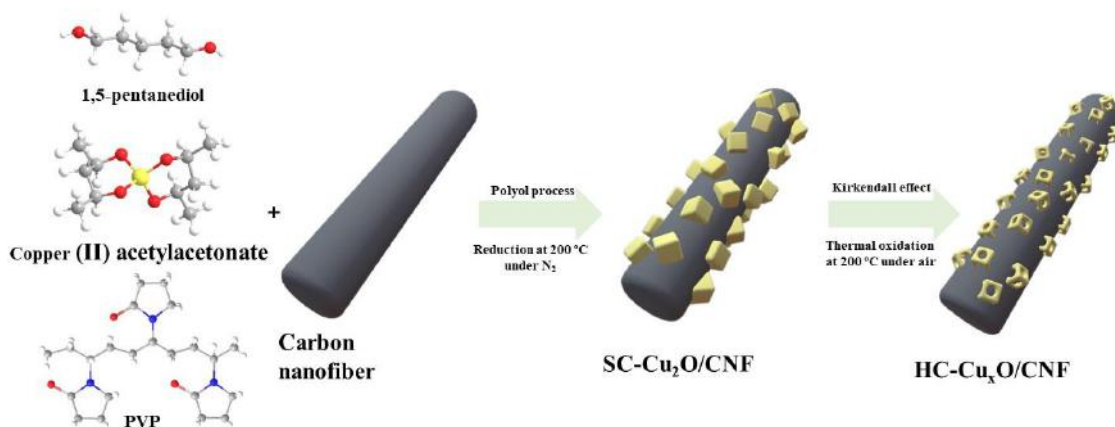


Controlled Synthesis and Uniform Anchoring of Hollow Cu_xO Nanocubes on Carbon Nanofiber for Enhanced Se(S)-Se(S) Bond Activation

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In the present study, we have constructed hollow cubic Cu_xO nanoparticles (~23 nm) incorporated with CNF (HC- Cu_xO /CNF) through controlled thermal oxidation of solid cubic Cu_2O nanoparticles (~21 nm) supported on carbon nanofibers (SC- Cu_2O /CNF) under airflow, exploiting the nanoscale Kirkendall effect. These hollow Cu_xO nanocubes with increased surface areas exhibited outstanding catalytic activity for unsymmetrical chalcogenide synthesis under ligand-free conditions.



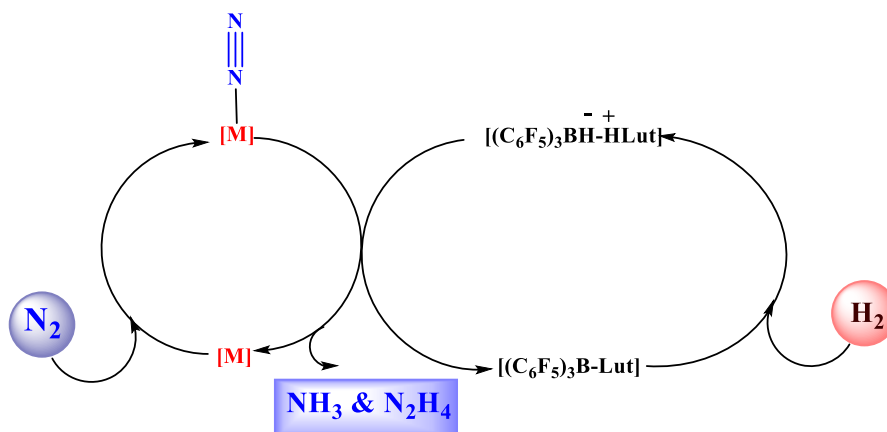
A brief synthetic scheme of HC- Cu_xO /CNF structure

Metal Catalysts for Nitrogen Activation & Reduction

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Ammonia is one of the most highly produced inorganic chemicals in the world, because of its utility as fertilizer, pharma industry, manufacture of nitric acid, nylon, polyamides, dyes, explosives and fuel etc.[1,2] Therefore, ammonia synthesis becomes more important, the most successful commercialized process for the synthesis of ammonia is the Haber–Bosch process, where the dinitrogen is reduced by dihydrogen in the gas phase under highly drastic reaction conditions using heterogeneous catalysts.[3] Nevertheless, the nitrogenase enzyme converts atmospheric dinitrogen into ammonia at ambient reaction conditions.[4] Several attempts have been made to discover a homogeneous catalyst for the nitrogen reduction into NH_3 . We have investigated the possibility of conversion of the coordinated dinitrogen into NH_3 and N_2H_4 using H_2 in the presence of Ru-triamidoamine and FLP (Frustrated Lewis pair) under mild experimental conditions.[5] We also attempted to demonstrate the functionalization of coordinated nitride (tpyOs(VI)-nitride) to ammonia using H_2 in the presence of phosphine (Lewis base).[6] We have studied metal borazine's reactivity towards dinitrogen molecules' activation by DFT calculations.[7] We have used the same method to determine the mechanism of ammonia and hydrazine synthesis using a molybdenum bound nitrogen doped graphene as a catalyst.[8]



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Poster Abstracts

P1

N-Nitrosuccinimide: Bench Stable Nitryl Radical Transfer Reagent

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Nitration reactions hold significant importance in organic synthesis and are foundational topics taught in schools. While the classical electrophilic nitration method using strong mineral acids prevailed for many years since its discovery in the 19th century, recent decades have seen a shift towards exploring new reactivity and reagents. Researchers now seek practical and mild reaction conditions for accessing nitro compounds. Organic nitrating reagents have emerged as key players in this endeavor, offering enhanced reactivity and enabling eco-friendly and sustainable nitration processes.¹ Herein, we present a novel dual photoredox-mediated paradigm for difunctionalization of alkenes, yielding challenging 1,2-halonnitroalkane molecules. We employ N-Nitrosuccinimide as a redox-active nitrating reagent to introduce a controlled amount of nitryl radicals into reaction mixture, while cobalt-mediated radical ligand transfer (RLT) facilitates the transfer of a secondary functionality into the organic scaffold. This synergistic process between photocatalyst and cobalt operates under mild conditions, enabling a one-pot synthesis of 1,2-chloronitro- and 1,2-bromonitroalkanes with excellent chemo- and regioselectivity, demonstrating exceptional functional group tolerance. Detailed mechanistic studies supported the role of cobalt as a radical halogen transfer catalyst. Furthermore, employing a net-neutral radical/polar crossover (RPC) approach under cobalt-free reaction conditions allowed to accommodate a variety of external protic nucleophiles, including thiols, alcohols, acids, and, notably, substituted amines.^{2,3} Highly functionalized olefin scaffolds also successfully underwent nitrative difunctionalization, demonstrating the viability of these protocols for the late-stage functionalization of bioactive molecules.

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Surface Enhanced Raman Spectroscopy for detection of dye on a novel Bismuth Substrates

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Surface-enhanced Raman Spectroscopy (SERS) study of new emerging non-noble bismuth semiconductor has attracted much attention in recent years. Non-noble bismuth substrates β - $\text{Bi}_2\text{O}_3/\text{Bi}_2\text{O}_2\text{CO}_3$ heterostructure nanoplates and $\text{Bi}_{24}\text{O}_{31}\text{Br}_{10}$ powders were synthesized through facile hydrothermal method via thermal treatment of $\text{Bi}_2\text{O}_2\text{CO}_3$ precursor and chemical precipitation method, respectively(1-2). The phase transformation of bismuth heterostructure was confirmed by shift in Raman peaks. While in case of $\text{Bi}_{24}\text{O}_{31}\text{Br}_{10}$ powders, the phase stability was confirmed by the relative Raman enhancement after the calcinations at different temperature. Moreover, the SERS activity of these novel substrates were performed by the detection of Methyl orange (MO), Rhodamine B (RhB), and 4-nitrophenol (4-NP). These probe molecules exhibit excellent SERS signal on both heterostructures with detection limit of 25 μM similar to the conventional substrates. The enhancement in Raman signal of probe molecule on bismuth substrate majorly governed by the chemical enhancement mechanism. Raman and SERS measurement were performed by 785 nm laser excitation source.

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Synthesis, Characterization of Metal-Organic Framework Based On Transition Metals for Antibacterial Activity and Dye Degradation Studies

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Metal-organic frameworks (MOFs) are innovative hybrid materials consisting of metal ions and organic bridging ligands with distinct coordination geometries. MOFs have gained significant attention in recent years due to their unique topology, optical characteristics, and framework design. 2,5-furan dicarboxylic acid (FDA) is a promising sustainable building material that can be produced from cellulosic biomass, making it a favorable alternative to materials that compete with food chains. This study successfully synthesized a 2D porous multifunctional Ni and Cu MOF using 2,5-furan dicarboxylic acid as organic linkers under hydrothermal conditions. The MOF was characterized using various methods such as Ultraviolet-Visible spectroscopy, FTIR spectroscopy, X-ray diffraction analysis, XPS spectroscopy, Scanning Electron Microscopy (SEM), and Transmission Electron Microscopy (TEM). This study determined the antibacterial efficacy of the synthesized Ni and Cu-MOFs against clinical and standard strains of gram-positive and gram-negative bacteria. The Ni and Cu MOFs were also demonstrated to be effective in environmental remediation by degrading a toxic dye, methylene blue (MB). The MOFs are non-toxic and safe to use as a catalyst to remove hazardous dyes without endangering the environment.

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Photodegradation Study of Evans blue in Presence of Cadmium Cobaltite

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The photocatalytic degradation of Evans blue under visible light was studied using cadmium cobaltite as the photocatalyst. Cadmium cobaltite was synthesized via a wet chemical precipitation method. The research evaluated the photocatalytic activity of cadmium cobaltite by comparing its effectiveness in degrading Evans blue dye. Various factors, such as pH, dye concentration, semiconductor amount, and light intensity, were analyzed to determine their influence on the degradation rate. The study found that cadmium cobaltite exhibited the highest catalytic activity in a basic medium. A tentative mechanism for the reaction has been proposed.

Keywords: Photocatalysis, Evans blue, Cadmium cobaltite, Degradation, Recyclability.

Synthesis, Characterizations and Biological Evolution of 1-Phenyl- N'-(3-phenylacryloyl)cyclopropane carbohydrazide Derivatives

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Cinnamic acid is the most common natural source of aromatic fatty acid from cinnamon bark, cocoa, grapes, celery, spinach, etc. It has a long history of human use as a component of plant-derived scents and flavouring agents. Cinnamic acid offers three main reactive sites: substitution on the phenyl ring, addition on the α , β -unsaturation and reactions of the carboxylic acid. It draws more attention to the biological activities of these derivatives in medicinal chemistry, such as antioxidant, anti-inflammatory, anticancer, antituberculosis, antifungal, antimalarial, and antimicrobial activities. Whereas carbohydrazide moiety also consists of many pharmaceutically available drugs like rimonabant (anti-Obesity), nitrofurantoin (urinary track infections), saluzide (treatment of tuberculous meningitis), carbazochrome (antihemorrhagic), nifuroxazide (antibiotic), dantrolene (spasticity), raltegravir (antiretroviral) etc. Cyclopropanamide is also a vital motif containing different biologically active compounds. In this paper, we synthesized two new compounds containing cinnamic acid groups, carbohydrazide, and cyclopropanamide groups in one compound. These 1-phenyl-N'-(3-phenylacryloyl)cyclopropane carbohydrazide derivatives are characterized by FT-IR, ¹H NMR, ¹³C NMR, elemental analysis and their biological evolution data are presented. These compounds possess distinct effective inhibition on the proliferation of U937, pro-monocytic, human myeloid leukaemia cell line, while these compounds did not show cytotoxic activity on these cells.

Ultrathin, Large Area β -Ni(OH)₂ Crystalline Nanosheet as Bifunctional Electrode Material for Charge Storage and Oxygen Evolution Reaction

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Bifunctional electrode materials are highly desirable for meeting increasing global energy demands and mitigating environmental impact. However, improving the atom-efficiency, scalability, and cost-effectiveness of storage systems, as well as optimizing conversion processes to enhance overall energy utilization and sustainability, remains a significant challenge for their application. Herein, we devised an optimized, facile, economic, and scalable synthesis of large area (cm²), ultrathin (~2.9±0.3 nm) electroactive nanosheet of Ni(OH)₂, which acted as bifunctional electrode material for charge storage and oxygen evolution reaction (OER). The β -Ni(OH)₂ nanosheet electrode shows the volumetric capacity of 2.82 Ah.cm⁻³ (0.82 μ Ah.cm⁻²) at the current density of 0.2 mA.cm⁻². The device shows a high capacity of 820 mAh.cm⁻³ with an ultrahigh volumetric energy density of 0.33 Wh.cm⁻³ at 275.86 W.cm⁻³ along with promising stability (30,000 cycles). Furthermore, the OER activity of ultrathin β -Ni(OH)₂ exhibits an overpotential (η_{10}) of 308 mV and a Tafel value of 42 mV dec⁻¹ suggesting fast reaction kinetics. The mechanistic studies are enlightened through density functional theory (DFT), which reveals that additional electronic states near the Fermi level enhance activity for both capacitance and OER.

Keywords: Ultrathin, 2D nanomaterials, Supercapacitor, OER. References

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Synthesis and Characterization of Iron and Cobalt based bimetallic MOFs and Immobilization in Alginate beads for the removal of Arsenic from water

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The decontamination of highly toxic arsenic (As) from aqueous environments using MOF granules has been an emerging area. Here we report a water stable bi-metallic MOF encapsulated alginate beads for the Arsenic remediation purposes. The MOF and alginate beads were characterized by powder XRD, SEM, TEM and BET surface areas measurement. Various Fe and Co based MOF-74 will be solvo-thermally synthesized by varying the ratio of metals. The Synthesized Fex-Coy-MOF-74 surface was modified by using the 0.5 M HCl. The Synthesized Fex-Coy-MOF-74 and as well as HCl modified MOFs will be further characterized using various spectro-photometric techniques such as FTIR, UV-vis, TGA, BET, SEM-EDS, TEM, P-XRD, SC-XRD, XPS and CHN analysis. Further Fex-Coy-MOF-74 will be applied for the Arsenic removal in batch process. In batch process dosage, concentration pH, temperature, effect of competing ions, reusability test, kinetics and isotherms will be studied thoroughly. Out of the various Fex-Coy-MOF-74 MOFs, the best MOF is further granulated using the sodium alginate. Finding out the optimum particle diameter for maximum adsorption by changing MOF ratio in the granulation process. After activation by HCl the granulated MOF is further used for the arsenic separation in batch as well as column process. Further Fex-Coy-MOF-74 will be applied for the Arsenic removal in batch process. In the batch process for the best granules, dosage, concentration pH, temperature, reusability test, kinetics and isotherms will be studied thoroughly. In Colum study breakthrough time, exhaustion time, reusability, effect of bed height, flow rate, and effect of arsenic concentration will be thoroughly studied for natural water. Finally, the best results will be used in pilot scale process.

Keywords: Arsenic removal; metal-organic frameworks; adsorption; granular adsorbents; water remediation.

Removal of Contaminants in The Effluent Water Using Bioremediation: A New Apotheosis Towards Waste Water Treatment

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The treatment of effluent water contaminated with various pollutants poses significant challenges to environmental sustainability. Bioremediation emerges as a promising approach, offering a sustainable and eco-friendly solution to mitigate the adverse effects of contaminants. This research investigates the efficacy of bioremediation techniques in removing pollutants from effluent water, focusing on its application as a novel paradigm in wastewater treatment. The study explores various aspects of bioremediation, including microbial diversity, metabolic pathways, and environmental factors influencing remediation efficiency. Through experimental analyses and field studies, the thesis evaluates the effectiveness of bioremediation in degrading specific contaminants such as organic pollutants, heavy metals, and nutrients. Furthermore, the research contributes to advancing bioremediation technologies by proposing innovative strategies and optimizing existing methods for enhanced contaminant removal. The thesis also considers the economic feasibility and scalability of bioremediation processes, addressing challenges and proposing recommendations for practical implementation in wastewater treatment facilities.

Overall, this thesis establishes bioremediation as a new apothecary in the realm of wastewater treatment, offering sustainable solutions to mitigate environmental pollution and promote water resource conservation.

Keywords: Bioremediation, Effluent water, Contaminant removal, Wastewater treatment, Environmental sustainability, Microbial diversity, Organic pollutants, Heavy metals

Thermally Stable Copolymers with Pendant “N-arylimide” Groups via Reversible Deactivation Radical Polymerization Technique

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Approximately 60% of synthetic polymers are currently prepared via free radical polymerization processes. Although, the conventional free radical polymerization methods have poor control over the molecular weight with broad polydispersity index making difficult to synthesize the polymers with desirable architectures. These limitations can be overcome by using reversible deactivation radical polymerization (RDRP) methods which is commonly known as 'controlled'/ 'living' radical polymerization. Among all RDRP methods, the atom transfer radical polymerization technique (ATRP) is more versatile due to their easy experimental requirements [1-2]. The “itaconimides” are the members of imide (-CO-NH-CO-) family with reactive exocyclic double bond and easily obtained from the renewable resource viz. D-glucose. The incorporation of imides such as itaconimides in the polymer backbone is reported to enhance glass transition temperature and thermal stability of resulting polymers [3].

In this work, we report the random and random-block copolymers of MMA with NAI monomers [such as (N-(4-chlorophenyl) itaconimide, Nphenylitaconimide, and N-(4-methoxyphenyl)itaconimide)] have been synthesized via AGET-ATRP method with “N-arylimide” as the pendant group and characterized by different techniques. A 60–80% enhancement in softening temperature of these copolymers was observed as compared to PMMA. These copolymers are potential candidates as ‘thermoplastics’ that can be used in a higher temperature range.

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Preparation of bio-adsorbent for the removal of Methyl orange dye

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Bio-adsorbent obtain from natural material like agricultural waste and microbial are eco-friendly and cost-effective. So, it is very interesting to discover its efficacy. However, the efficiency of bio-adsorbent depends on its modification techniques. This study aim is to compare all the modification and activation methods of bio-adsorbent and heir characterization, the removal efficiency of Methyl orange by the use of the effective modified bio-adsorbent, to do the isotherm and kinetics study and to provide valuable insight for future research and application in environmental remediation practices.

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The Oxygen Vacancies Induced Local Surface Plasmon Resonance for NIR Shielding in Titanium - Tungsten Oxide Doped Borosilicate Glasses

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The global energy demand is going to increase manifold in coming years. To meet future energy requirements, we need to save energy by all the means. The main perspective of the present work is to synthesize cost-effective borosilicate glasses which were synthesized for NIR-shielding application. NIR shielding energy saving glass system was prepared by conventional melt quenching method. The chosen chemical composition is $xWO_3 + (27 - x)Na_2O + 38.7B_2O_3 + 34SiO_2 + 0.3TiO_2$ (where $x = 0, 1, 2, 3, 4$ and 5 mol%). The X-ray diffraction (XRD), UV-Vis NIR and Raman spectroscopy were employed to evaluate the structural and optical properties of titanium-tungsten oxide doped borosilicate glasses, respectively. X-Ray Photoelectron spectroscopy (XPS) confirmed the chemical states of the tungsten in the glasses. The glass having $x=3$ mol% of WO_3 and 0.3 mol% of TiO_2 borosilicate glass (BSG 3) is found to have good NIR shielding ability ($T_{min} \sim 77.3\%$ at 2217 nm) with acceptable visible light transmittance ($T_{max} \sim 90.4\%$ at 772 nm), and hence proposed for applications in NIR-shielding energy-saving windows. The present study emphasizes on tunable NIR-shielding performance of synthesised energy-saving glasses. The optimized glass composition can be taken from lab to industrial application and many more endeavors for the manufacturing of energy saving glasses. The glass having $x=3$ mol% of WO_3 and 0.3 mol% of TiO_2 borosilicate glass (BSG 3) is found to have good NIR shielding ability ($T_{min} \sim 77.3\%$ at 2217 nm) is attributed to titanium-tungsten oxide incorporation in glass network. The energy saving glasses, transparent to visible light and having NIR shielding, can be used in glass windows of industry buildings, houses, and motor vehicles to reduce the load on air conditioners.

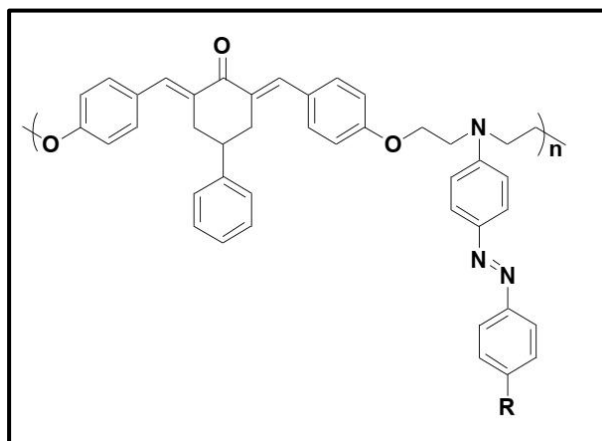
Keywords: Near infrared shielding, Visible transmittance, Local surface plasmon resonance, nonstoichiometric tungsten oxide, Oxygen vacancies.

NLO Polymer Synthesis and Characterization: A Review

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Materials used in nonlinear optics (NLO) include inorganic crystals, organic small molecules and polymers. These materials have a wide range of uses, such as frequency generating, optical data storage, and optical communication. Scientists are working to create organic polymers with many advantages over inorganic and organic small molecules. The primary issue with NLO active polymers for applications is their stability, which can be fixed by making the polymer chain more rigid. The overall plan focuses on creating synthetic pathways through several methods in which monomers are chemically joined to a polymer as a side chain or integrated into the main chain, as illustrated below. Using a Nd:YAG laser (1064 nm), the NLO activity in the polymer is confirmed for use.



Utilization Of Agri-Waste for Developing Freestanding Membrane for Forward Osmosis Application.

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In order to explore the new frontier of futuristic technology in the field of water purification, biodegradability is a crucial aspect in the development of contemporary membranes as an environmentally benign substitute for synthetic membranes already on the market. This work developed, for the first time, free-standing, biodegradable, sustainable Forward Osmosis (FO) membranes based on sugarcane bagasse-derived cellulose (SBC) that can produce high quality water. In this work, a readily recoverable ethylenediaminetetraacetic acid disodium (EDTA-2Na) solute can be used as a draw solution (DS) component to achieve dewatering. The optimised FO membrane performs admirably, as evidenced by the osmotic flux of clean water and reverse solute flux (RSF), which both have retention rates of roughly >99% for all contaminants. Three separate attempts were made to recover DS, with >85.68% and >84.56% flux retention for pure water and industrial effluent, respectively, as feed solutions. About 99% retention of organic and other foulants with long-term stability was observed for the simulated wastewater made up of several pollutants. By mulching in the soil for three weeks, membranes' capacity to decompose naturally was further investigated. Therefore, these membranes were ideal building blocks for the forward-thinking creation of environmentally safe and sustainable water purification techniques in the FO process.

Keywords: sustainable development, biodegradability, forward osmosis, freestanding membrane.

Sustainable Carbon Dots from *Borreria hispida*: Enhanced Colorimetric Sensing of Fe³⁺ Ions and Biological Applications in Live Cell Imaging

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This study presents the synthesis of advanced nanomaterials derived from the Hedge-grown herbal plant, *Borreria Hispida*, and explores their environmental and biological applications. Using a one-step hydrothermal synthesis method, carbon dots derived from *Borreria Hispida* (BHCD) were fabricated and thoroughly characterized through XRD, TEM, FTIR, CHNS, UV–visible, and PL spectroscopy analyses. Under UV illumination, these plant-based carbon dots demonstrated exceptional water solubility, notable photo stability, and a high quantum yield of 40.8%. The average particle size of BHCD was absorbed around 0.5 to 3.5 nm, contributing to superior selectivity and sensitivity in detecting Fe³⁺ ions, with a limit of detection of 1.2 × 10⁻⁶ M. Investigation into the sensing mechanism revealed a binding model wherein two carbon atom molecules bind to one Fe³⁺ atom in a 2:1 ratio for BHCDs and Fe³⁺ interactions. Additionally, the effectiveness of the developed fluorescent probe for Fe³⁺ detection was validated using real water samples from ponds and lakes, highlighting its potential for environmental monitoring applications. Furthermore, the biological effects of BHCD were evaluated through cytotoxic assays, demonstrating significant inhibitory effects on MCF7 breast cancer cell lines, with a maximum cell viability of 60%. This research underscores the multifaceted potential of BHCD in environmental monitoring and biomedical applications.

Fenton-Like Catalysts Based on Graphitic Carbon Nitride Nanosheets Decorated with Fe₃O₄ Nanoparticles for Removal of Colorless Tetracycline

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Widespread usage of colorless pharmaceutical drugs in our daily lives leads to an accumulation in the level of water bodies and potable water, resulting in a variety of adverse health effects when consumed unknowingly. So, it is of utmost importance to remove these types of contaminants from effluent. In this work, an in-situ synthetic strategy was implemented for the preparation of nanocomposite consisting Fe₃O₄ nanoparticles decorated on metal-free graphitic carbon nitride (FCN) and employed for the degradation of colorless tetracycline (TC) by heterogeneous Fenton-like reaction. The presence of Fe²⁺ and Fe³⁺ in the nanocomposites led to active participation in the Fenton-like reaction and the formation of reactive oxygen species responsible for TC degradation. It was observed that a maximum of 90 % of TC got degraded within 60 minutes in the case of FCN-20 %. A radical scavenging study revealed the direct involvement of superoxide radicals (O₂⁻) and singlet oxygen (¹O₂) for efficient degradation. The nanocomposite also showed a significant removal rate of TC in real water samples. It was worth noticing that the catalyst exhibited exceptional magnetic properties with good reusability and insignificant changes after reuse. The formation of small molecules from the degradation of TC was identified via high-resolution mass spectroscopy (HR-MS). This catalyst will show promising application for the removal of organic contaminants in aqueous environment.

Exploring the Synergistic Effect of Aggregation and Hydrogen Bonding: Fluorescent Probe for Dual sensing of Phytic Acid and Uric Acid

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We synthesized an unoxidized bis-indolyl methane (BIM) derivative (probe 1) comprising tetraphenylethylene (TPE) as the signalling moiety. The amphiphilic probe could form self-assembled nanoscopic aggregates in the aqueous medium. The fluorescence response of 1 in non-polar solvents originates from LE state, while in polar solvents, it is dominated by TICT. Moreover, probe 1 exhibited 'turn-on' fluorescence response for both uric acid (with blue shift in emission maxima) and phytic acid (with red shift in emission maxima). Therefore, the present system provides an exceptional opportunity to distinguish between phytic acid and uric acid by considering two different emission channels. The mechanistic investigations revealed that both H-bonding and electrostatic interactions between the probe and analytes could effectively cause restricted intramolecular rotations, leading to turn-on response. Additionally, in the case of phytic acid, larger aggregates were observed with prominent CT characteristics. The change in the extent of charge transfer interaction in the formed adducts, resulted in distinct fluorescence responses with phytic acid and uric acid. Further, we explored the applicability of the present system in the screening of real-life samples, such as uric acid in urine sample and phytic acid in grains. The LOD for phytic acid and uric acid was found to be ~5.48 nM and 10.4 nM. The quantitative nature of the system was confirmed, showing promising results in terms of recovery values (between 95.6-104.2 %) and detection limits. Additionally, we also employed handy paper strips for the on-site monitoring of phytic acid and uric acid, eliminating the need for complex instrumentation or trained technicians.

Synthesis of Organic and Organic-inorganic Hybrid π -conjugated Semiconducting Materials for Optoelectronic Devices

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Organic solar cells (OSCs) have attracted much attention due to several technological advantages of light weight, flexibility, large-area fabrication via simple solution deposition techniques. The development of novel photoactive materials and device engineering in the last few years, the power conversion efficiencies (PCEs) of OSCs have currently reached over 19% for single-junction cells,[1] demonstrating their great potential in future applications. The major problem of biphasic bulk-hetero junction (BHJs) solar cell is the optimized morphology is thermodynamically unstable and the progressive macrophase separation of donor (D) and (A) leads to a decrease of PCE and stability of OSCs.[2] Therefore, control of the active layer morphology is an important parameter for realizing good performance and stable commercially viable OSCs. Single material organic solar cells are an important alternative to make large scale organic solar cells, are composed of only one organic material that serves as both the light-absorbing layer and the charge transport layer, eliminating the need of complex device architectures and multiple interfaces that can cause performance degradation and device instability. On the other hand, Two-dimensional (2D) organic-inorganic hybrid perovskites, which incorporate functional organic cations, have emerged as a new type of semiconducting material useful for optoelectronic devices such as solar cells, LEDs, and photodetectors. We studied a lead-based 2D perovskite structure, Dion-Jacobson type, incorporating simple terphenyl diammonium salts as organic spacers. Type II heterostructures formed by organic semiconducting ligands and in 2D perovskites can offer separated charge transport channels for holes and electrons. This work gives valuable insights into the charge transport mechanisms of type II heterostructures and paves the way toward optoelectronic device applications for such Dion–Jacobson-type 2D perovskites.

Keywords: Renewable energy, organic solar cells, π -conjugated materials, 2D dion-jacobson perovskite, p-n heterojunction, charge transport properties

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Design, synthesis, crystal structure analysis, Hirshfeld surface scrutiny, and quantum mechanical calculations of fused 4H-pyrans and spirooxindole-embedded fused pyran scaffolds!

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Fused 4H-pyrans and spirooxindoles are crucial heterocycles that form the backbone of many natural products and medicinally significant molecules. In this study, we synthesized and examined a variety of pyrano[3,2-b]pyran and spirooxindole molecules. The structures of these compounds were confirmed by X-ray diffraction. The fused 4H-pyran molecules crystallized in monoclinic and triclinic systems, specifically in space groups P-1, P21/c, and P21/n. The spirooxindole molecule crystallized in the tetragonal space group P42/n, featuring a single unique molecule in its asymmetric unit. Hirshfeld surface analysis revealed intermolecular interactions within the crystal structures. Additionally, we optimized the molecular geometry of all compounds using the DFT method with the B3LYP hybrid functional and 6-311+G(d,p) basis set, which aligned well with experimental results. An electrostatic potential map was created to highlight the energy distribution and reactive regions of the molecules.

Growth and characterization optical studies of N-acetyl-L-alanine A potential optoelectronic NLO material

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The single crystal of N-Acetyl-L-alanine (NALA) has been synthesized by slow evaporation growth technique at ambient temperature using aqueous medium. The unit cell parameters of NALA crystal were identified using single crystal XRD analysis. The various functional groups in the crystal can be identified by FTIR analysis. The Ultraviolet-visible analysis used to prove the cutoff wavelength 231 nm of the crystal, Urbach energy calculated value of 0.11 eV and various optical constant values supports the NLO nature of NALA crystal. Wemple-DI Domenico model used to determine the various single oscillator parameters. Surface analysis and the various elements present in this NALA crystal is proved by SEM with EDAX analysis. The SHG studies proves the 1.4 times greater efficiency of NALA crystal than the KDP. Mechanical studies proved by vicker microhardness studies. RISE pattern has been validated by making used of the theoretical models proposed by Meyer and Hays – Kendall. Thermal stability of the crystal is proved by TG and DTA analysis. Glass transition (T_g) temperature proved by DSC analysis. Thermodynamic parameters elucidated by using the Redfern method. N-methylation is the derivatives reside to methyl amide of N-acetyl L-alanine having the limitation in the freedom related to confirmation of the peptide chain. The shape owe to the potential surface is utmost sensitive towards the position of N-methyl group and its orientation related to the basic chain. Nitrogen substituted amino acid confirms the importance of hydrogen bonding. The molecular structure of NALA is shown in Fig.Molecular structure of N-acetyl-L-alanine

Keywords: N-Acetyl L-alanine, SHG, UV analysis, Wemple-DI Domenico model, Redfern method.

Detection of Date Rape Drugs Using Biomolecules

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Proteins can also act as recognition elements in sensor devices where the protein is attached to a solid support and the combined unit acts as a transducer of an optical signal. There has been long-standing interest in the development of such sensors in the environmental, chemical, and medical sciences for the detection of a variety of analytes, as well as more recently for the detection of chemical and biological warfare agents. Ideally such sensor devices should be portable, rapid, and straightforward to use. Where proteins are employed in the sensing elements, there continues to be the need for attachment methods that ideally preserve or increase the stability of the immobilized protein, since such devices may be stored for prolonged periods before deployment and must be sufficiently robust for field use.

Keywords: Protein, solid support, attachment method, sensor, optical signal

Synthesis of Chiral β -Aminoketones via Encapsulated Chiral Zn(II)–Salen Complex

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In order to achieve sustainable chemical transformations, eco-friendly approaches are essential in conjunction with economic growth and environmental conservation. In present study a greener decorum for synthesizing distinctive Zn(II)-Salen complex encapsulated in MWW host as a heterogeneous chiral catalyst, i.e., Zn(II)-Salen@MWW. A variety of techniques were used to substantiate the chiral Zn(II) complex' encapsulation, including FTIR, FESEM, EDX, XRD, BET, and XPS. Using an unpretentious ultrasonic approach, the synthesized catalyst could effectively generate chiral β -amino carbonyl compounds at room temperature under solvent-free condition. There are multiple advantages to using this protocol, including a green and efficient catalyst, a simple set-up procedure, effortless separation, and the ability to reprocess up to five runs of the chiral Zn(II)-Salen@MWW catalyst. There is a high likelihood that this process will be beneficial both in academia and industry.

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Chitosan-palladium nanocomposites for organic transformations: A brief study

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Chitosan, a natural biopolymer with a modifiable structure and abundant function groups, can be processed into various shapes and sizes. Additionally, the biocompatibility of chitosan makes it researchers' preferred material for exploration. This chitosan can be modified through physical, chemical, and biological modifications, to obtain versatile chitosan-based materials. These chitosan-based materials can be fabricated into different shapes and sizes, such as nanofiber, nanoparticles, microspheres, membranes, and 3D printed scaffolds, making it suitable for various applications. On the other hand, palladium (Pd), though an expensive precious metal, has displayed its versatility in organic transformations both as complexes and nanoparticles (NPs). However, the impaired recovery of the homogenous catalyst, while the decline in catalytic activity due to agglomeration in bare Pd NPs are some of the greatest limitations of Pd-based systems. A feasible strategy to overcome these shortcomings, is the heterogenization of the Pd system onto a suitable inert heterogeneous support material, herein chitosan-based materials. Thus obtained chitosan-Pd nanocomposite improves the dispersion of the catalytically active Pd and the almost full recovery of the nanocomposite. This work provides an insight into some of the recent chitosan-Pd nanocomposites developed for a choice of organic transformations. The synthetic approach, characterization, applications and recyclability are discussed to provide a bird's eye view of these chitosan-Pd nanocomposites.

Keywords: Chitosan; Palladium; Nanocatalyst; Organic transformations; Green

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Selective Cyanide Ion Detection Using Hydrazine Carbothioamide Probe: A Fluorescence Turn-On Approach

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The synthesis of various hydrazine carbothioamide derivatives via Schiff base reactions, confirmed by FT-IR, NMR (¹H and ¹³C), and HRMS spectroscopic methods. Among these derivatives, probe L ((4-fluorobenzylidene)-2-(1-phenylethylidene)hydrazine-1-carbothioamide) emerged as a highly selective fluorometric chemosensor. Detailed absorbance and emission spectra analysis that probe L exhibits a specific turn-on fluorescence response to CN⁻ ions with minimal interference from other anions. Job's method confirmed a 1:1 binding stoichiometry between probe L and the revealed cyanide ion. The detection limits (LOD) and quantification limits (LOQ) were determined to be 0.639 μM and 2.116 μM, respectively. The detection mechanism was elucidated using FT-IR spectroscopy, ¹H NMR titration, and HRMS. Additionally, probe L demonstrated effective CN⁻ ion detection in water and food samples, underscoring its potential as a practical sensor for cyanide detection.

Targeted Phototriggered Drug Delivery by a System of Di-block Copolymer and Spiropyran Micelles with Real-time monitoring through the NSET Mechanism

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A Photo-responsive drug delivery system based on polymeric micelles has been formulated, utilizing easily available and cost-effective materials such as an amphiphilic diblock copolymer and a Spiropyran derivative. This system addresses the major challenges in drug delivery systems i.e., monitoring real-time drug release, targeted, and on-demand drug delivery. To monitor real-time drug release, we incorporated AuNPs into the micellar nanocarrier via in-situ synthesis where, the fluorescence quenching of the cancer drug, Doxorubicin by AuNPs was explored through the Nanomaterial Surface Energy Transfer (NSET) mechanism. Photochromism and size switching were characterized using UV-Vis spectroscopic and dynamic light scattering (DLS) techniques. The energy transfer process during in-situ synthesis of AuNPs and drug release after 365 nm UV light exposure of nanocarrier has been demonstrated by steady-state and time-resolved fluorescence of DOX. The DOX-mPEG PLA-Spiropyran (1:3:1) formulation exhibited an encapsulation efficiency of ~73.16% and a DOX-loading of ~ 6.45%. This formulation was stable as proven by a kinetic stability study. Moreover, they showcased the sustained DOX release for over 50 hours, validated by In vitro drug release studies. Cell internalization, intracellular photo-triggered drug release, and fluorescence cell imaging in Mouse breast adenocarcinoma cells (4T1) cells have been investigated. The results demonstrated that the DOX-mPEG PLA-Spiropyran micelles after 365nm UV light exposure were highly efficient in inducing apoptosis, significant cytotoxicity, and mitochondrial membrane depolarization. Overall, our study demonstrates the efficacy of this drug delivery system for cancer treatment, enabling targeted, on-demand drug delivery with real-time monitoring of drug release through the NSET mechanism.

Keywords: Photochromism, Monitoring Real-time drug release, Targeted on-demand drug delivery, mPEG-PLA, Spiropyran Photo

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Mapping the Journey of Biomolecules: Exploring SERS Investigation

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The use of Raman and surface-enhanced Raman spectroscopy (SERS) for disease detection has garnered significant attention in recent decades. SERS is highly regarded for its exceptional sensitivity and non-destructive nature, enabling the generation of distinct vibrational spectra for surface species, even at the level of individual cells and molecules. This powerful platform offers the potential to visualize internalization processes and monitor therapeutic effects, addressing the complex challenge of understanding mechanistic events. In one of our studies, we developed a theranostic probe using spherical and hollow gold nanoparticles, demonstrating its application in deciphering biomolecular events. The specifically designed spherical gold nanoprobe was employed to trace internalization and microtubule disruption events associated with the non-fluorescent drug paclitaxel (PTX). Additionally, we conducted another study utilizing SERS fingerprinting and imaging to observe the effects of a targeted theranostic platform using innovative hollow gold nanoparticles. This approach allowed us to monitor the molecular-level therapeutic progression of combination therapy in cells and spheroidal models. The promising findings and analytical validation presented in this research represent crucial steps toward clinical validation, highlighting the potential of SERS in biological applications.

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Meta-Analysis of the Motor Protein KIF14 with Reference to Cancer

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It is anticipated that comprehensive genomic profiling will revolutionize cancer treatment. In a variety of cancers, tumorigenesis is caused by KIF14 signaling. In this perspective, we discuss the prevalence of copy number changes and KIF14 mutations in various solid tumors. We utilized significant data sets like cBioportal, PubMed, and COSMIC for KIF14 transformation and enhancement information assortment from different tumors. The clinical data for a variety of cancers caused by the KIF14 (kinesin family member 14) mutation are detailed in our results. Area of interest change of human KIF14 protein uncovers that more than once and most transformed locales and these areas of interest might be a symptomatic device for malignant growth affirmation. The prevalence of amino acid and nucleotide changes was reported in several distinct cancers. In this review, however, we all present the amino acid and nucleotide changes in various cancers. The missense mutation is the most common in all types of cancer, as demonstrated by our data collection on the KIF14 mutation and its distribution in various cancer tissues.

Keywords: Receptor threonine kinase; KIF14, Protein regulating cytokinesis 1; Citron kinase; motor protein; lung cancer.

Cyclometalated Ir(III) Complexes Bridged by μ -OH and μ -3,5-Bis(4-methoxyphenyl)-Pyrazole Ligands*Mausami^a, Harshit^a Trivedi^a, Bani Mahanti,^{*a}**^a Chemistry Section, Mahila Mahavidyalaya, Banaras Hindu University, Varanasi-221005*

The rich and diverse chemistry displayed by mononuclear to multinuclear Cyclometalated Iridium(III) complexes, which possess efficient triplet emitter characteristics, has propelled this class of compounds into the spotlight [1-3]. Several experimental and theoretical investigations have delved into cyclometalated Ir(III) complexes, elucidating fundamental principles for tuning emission color by variation of the ligands. While existing methods, involving electron-donating or withdrawing substituents, have been extensively documented for phosphorescence color tuning, there remains a strong impetus to devise phosphors with easily modifiable emitting properties through modifications of the electronic structure of both cyclometalating and ancillary ligands. The persistent motivation driving research in this field stems from the rich photophysical properties exhibited by these complexes [4]. Herein, we report the synthesis, characterization, photophysical and electrochemical studies of heterobridged cyclometalated organometallic Ir(III) dimers, [(ppy)₂Ir(μ -OH){ μ -(PhOMe)₂Pz}]Ir(ppy)₂] (1), [(tpy)₂Ir(μ -OH){ μ -(PhOMe)₂Pz}]Ir(tpy)₂] (2) (ppyH = 2-phenylpyridine; tpyH = 2-para-tolylpyridine; (PhOMe)₂PzH = 3,5-bis(4-methoxyphenyl)-pyrazole). Both these complexes are found to be emissive in nature. Additionally DFT and TDDFT studies have been performed to gain insight about the photophysical properties

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Detection of AsO_2^- And PO_4^{3-} Ions: Design and Key Properties

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In the quest for advanced analytical tools, we present a groundbreaking thiophene-based chemosensor engineered for the discriminative detection of arsenite (AsO_2^-) and phosphate (PO_4^{3-}) ions. Thiophene, a conjugated heterocyclic compound known for its exceptional electronic properties, forms the core of our sensor design, enhancing its sensitivity and selectivity for target ions. The synthesized probe was subjected to confirmation of the structural arrangement by NMR, LCMS, and FTIR analysis. The TPNH chemosensor exhibited selectivity and specificity towards AsO_2^- , and PO_4^{3-} ions over other common ions in semi-aqueous media (DMSO: water, 6:4, v/v)^{1,2}. The receptor TPNH distinguishes the selective ions based on their visible color change from yellow to green in presence of AsO_2^- and yellow to blue in presence of PO_4^{3-} ions. The Detection limit of 2.86 ppm for AsO_2^- and 5.16 ppm for PO_4^{3-} ions demonstrates the effectiveness of sensors towards arsenite. The B-H plot suggests that the binding constant and stoichiometric ratio as 1:1 between the TPNH and other active ions. The results were further supported by the UV-visible titration, electrochemical studies, ¹H NMR titration analysis and DFT validation, which promoted the mechanism of the sensor binding with the ions by Intramolecular Charge Transfer (ICT). Finally, the prominent sensing properties of TPNH aided the test strip application, and logic gate operations.

Chemosensor	Binding constant (M^{-1})	Detection limit (LOD)(ppm)	Stoichiometric Ratio
TPNH+ AsO_2^-	7.204×10^3	2.869	1:1
TPNH+ PO_4^{3-}	8.952×10^3	5.160	1:1

References

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Green and Ecofriendly Approach to Alternatives of Wound Dressing Materials

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