



One Day International Seminar
On

# EMERGING TRENDS IN SCIENCE AND TECHNOLOGY

Date: 23rd May, 2025

Organised By
Department of Chemistry
Kharagpur College

Kharagpur, Paschim Medinipur, West Bengal, India

# **ABSTRACT**



### **Program details**



### One day International Seminar

### EMERGING TRENDS IN SCIENCE & TECHNOLOGY

Organised by

Department of Chemistry

Kharagpur College

Kharagpur, Paschim Medinipur, West Bengal, India 721305

Date: 23<sup>rd</sup> May, 2025: Venue: H. B. Sarkar hall, Kharagpur College

#### **Speakers**



Prof (Dr.) Amit Kumar Das Professor Bioscience and Biotechnology, Indian Institute of Technology, Kharagpur



Dr. Subhash Chandra Ghosh **Principal Scientist** Marine Natural Products & Bio Polymer Division Associate Professor (Ac-SIR-New Delhi) CSIR- Central Salt & Marine Chemicals Research Design and Manufacturing, Jabalpur.



Dr. Amaresh Chandra Mishra Assistant Professor Department of Natural Sciences, PDPM Indian Institute of Information Technology,



Dr. Milan Pramanik Alumnus. Kharagpur College Postdoctoral Research Associate Cardiff University, U.K.

### Organising Committee

Chairman: Dr. Bidyut Samanta, Principal, Kharagpur College

Organizing Secretary: Smt Kuheli Pramanik, Assistant Professor & Head, Department of Chemistry

Jt. Secretary: Dr. Forid Saikh, Assistant Professor, Department of Chemistry & Sri Sanjoy Kumar Bera, SACT, Department of

Jt. Convener:Dr. Subhra Mishra & Dr. Indranil Chakraborty, Associate Professor, Department of Chemistry, Kharagpur College

#### Advisory committee

Dr. Gagan Chandra Mandal, Associate Professor, Department of Chemistry, Kharagpur College

Sri Prasanna Kumar Duley, Assistant Professor, Department of Chemistry, Kharagpur College

### Technical subcommittee

Jt Convener: Dr. Sumit Kumar Ray, Assistant Professor & Sri Kalyan Sur, SACT, Department of Chemistry, Kharagpur

#### College

### Reception Subcommittee

Convener: Smt. Laboni Giri, SACT, Department of Chemistry, Kharagpur College



### PROGRAMME SCHEDULE

Registration (9.30 am - 10.30 am)

**Inaugural Session** (10.30 am -11.00 am)

Welcome address: Dr. Bidyut Samanta, Principal& Patron in Chief, Seminar Organizing Committee

Speech by **Smt. Kuheli Pramanik**, Head, Department of Chemistry & Organising Secretary Speech by **Dr. Jagomohan Acharya**, In Charge Morning Shift, Kharagpur College Speech by **Dr. Abinsah Sengupta**, Secretary, Teachers' Council, Kharagpur College Vote of thanks by **Dr. Subhra Mishra**, Joint Convener, Seminar Oranising Committee

### **Technical session-1**

**Key Note Address:** (11.10 am- 11.50 am)

Speaker: Prof. (Dr.) Amit Kumar Das

Professor, Bioscience and Biotechnology, Indian Institute of Technology, Kharagpur, West Bengal

**Topic: New Trends in Structural Biology** 

Chair: Dr. Subhash Chandra Ghosh, CSMCRI, Bhabnagar

**Invited Lecture 1**(11.50 noon 12.30 pm)

Speaker - Dr. Subhash Chandra Ghosh

Principal Scientist, CSIR- Central Salt & Marine Chemicals Research Institute, Bhavnagar Associate Professor (AcSIR-New Delhi), CSIR-Central Salt and Marine Chemicals Research Institute

Topic: Regioselective C-H Activation: A Strategic Approach to Functionalized Arenes and Aldehydes

Chair: Prof. (Dr.) Amit Kumar Das, Professor, IIT, Kharagpur

### 12.30 pm- 1.30 pm: Lunch break & Postering Session

### Chair: Sri Kalyan Sur, Sri Sanjoy Kumar Bera & Smt Laboni Giri, Kharagpur College Paper Presenter

- 1. Dr. Kousik Bhattacharya, State Aided College Teacher, Department of Mathematics, Kharagpur College
- 2. Dr. Mukul Maity, State Aided College Teacher, Department of Geography, Kharagpur College
- **3.** Dr. Barnali Jana, Assistant Professor of Chemistry, Government General Degree College, Keshiary.
- 4. Sudipta Manna, Student, 3<sup>rd</sup>Sem, Department of Chemistry, Kharagpur College.
- **5.** Arpan Palmal, Student, 3<sup>rd</sup>Sem, Department of Chemistry, Kharagpur College.
- 6. Susmita Shit, UG student, Chemistry, Midnapore City College
- 7. Arindam Sahoo, UG student, Chemistry, Midnapore City College
- 8. Dr. Indranil Chakraborty, Associate Professor of Chemistry Kharagpur College.
- 9. Dr. Ipsita Kumar Sen, Assistant Professor of Chemistry, GGDC, Salboni
- 10. Dr. Ritwik Saha, Assistant Professor of Physics, Kharagpur College.



- 11. Jayanta Murmu, Assistant Professor of English, Kharagpur College.
- 12. Soumyabrata Sil, Assistant Professor of English, Kharagpur College.
- 13. Dr. Forid Saikh, Assistant Professor of Chemistry, Kharagpur College.
- 14. Kuheli Pramanik, Assistant Professor of Chemistry, Kharagpur College.
- 15. Dr. Sumit Ray, Assistant Professor of Chemistry, Kharagpur College.
- 16. Kalyan Sur, SACT, Department of Chemistry, Kharagpur College.
- 17. Sanjoy Kumar Bera, Research Scholar, Dr. C.V. Raman University, Vaishali, Bihar, SACT, Department of Chemistry, Kharagpur College
- 18. Amit Roy, Librarian, Kharagpur College.
- 19. Mihir Das, Assistant Professor of Physics, Kharagpur College.
- 20. Alok Haldar, Assistant Professor of Computer Science & BCA, Kharagpur College
- 21. Susanta Kumar Giri, Assistant Professor of Chemistry, Garbeta College.
- 22. Lakshmikanta Das, Assistant Professor of Chemistry, DGDC Kharagpur-II

### **Technical Session- 2 (Virtual mode)**

### **Invited Lecture 2 (1.30 pm - 2.10 pm)**

### Speaker: Dr. Milan Pramanik

Postdoctoral Research Associate, School of Chemistry, Cardiff University, United Kingdom Topic: From Bonds to Benefits: Sulfur-Containing Molecules in Organic Synthesis and Technology

Chair: Dr.Forid Saikh, Kharagpur College

### Invited Lecture 3 (2.10 pm-2.50 pm)

### Speaker: Dr. Amaresh Chandra Mishra

Assistant Professor, Department of Natural Sciences, PDPM

Indian Institute of Information Technology, Design and Manufacturing, Jabalpur

Topic: Magneto Impedance Effect in Electrodeposited Wires for Sensor Applications

Chair: Dr. Forid Saikh, Kharagpur College

### Oral presentation by participants (2.50 pm onwards)

(Duration of each presentation: 08 minutes)

## Chair: Dr. Gagan Chandra Mandal and Dr. Sumit Kumar Roy, Kharagpur College Paper presnter:

- 1. Happy Das, State Aided College Teacher, Kharagpur College.
- 2. Dr. Totan Ghosh, Assistant. Professor of Chemistry, MAKAUT.
- 3. Uttam Das, Assistant Professor of History, Kharagpur College.
- 4. Chandan Das, Research Scholar, IIT Bombay (Online).
- **5.** Dr. Ananya Das Mahapatra, Asst. Professor of Biotechnology, Brainware University (Online)
- **6.** Dr. Amrita Chakraborty, Assistant Professor of Chemistry, A. N. College, Patna, (Online)
- 7. Shaon Dey, SRF, IIT (ISM), Dhanbad (Online)
- 8. Dr. Abul Kalam Biswas, Assistant Professor of Chemistry, Mahishadal Raj College



(Online)

- 9. Dr. Shalmali Hui, Assistant Professor of Chemistry, Hijli College (Online)
- 10. Rudra Narayan Mondal, Assistant Professor of Physics, Kharagpur College (Online)
- **11.** Dr. Sukla Nandi, Assistant Professor, Chandrakona Vidyasagar Mahavidyalaya. (Online)
- **12.** Dr. Soumya Sundar Mati, Assistant Professorof Chemistry, Government General Degree College, Singur. (Online)
- 13. Pranim Rai, Assistant Professorof Economics, Kharagpur College. (Online)
- 14. Dr. Sushovan Paladhi, Assistant Professor of Chemistry, T.P.S. College, Patna
- 15. Jayanta Shounda, Assistant Professor of Mathematics, IAE, Hydrabad. (Online)
- **16.** Dr. Shib Shankar Dash, Assistant Professor of Chemistry, Ramkrishna Mahato Government Engineering College. (Online)
- 17. Chinmoy Mondal, Assistant Professor of English, Kharagpur College (Online)

### Valedictory session

5.30 pm

Vote of thanks: Dr. Forid Saikh, Kharagpur College



### From the desk of the Principal

Good morning, everybody.

Respected key note speaker of today's seminar Prof. (Dr.) Amit Kumar Das, Professor, Bioscience and Biotechnology, IIT, Kharagpur, respected resource persons, Dr. Subhash Chandra Ghosh, Principal Scientist, CSIR- Central Salt & Marine Chemicals Research Institute, Bhavnagar, Dr. Milan Pramanik, An alumnus of department of Chemistry of our college, presently working as a Postdoctoral Research Associate, Cardiff University, United Kingdom, Dr. Amaresh Chandra Mishra, Assistant Professor, Department of Natural Sciences, PDPM Indian Institute of Information Technology, Design and Manufacturing, Jabalpur, Dr. Jagomohan Acharya, In-Charge, Morning shift, Dr. Abinash Sengupta, Secretary, Teachers' Council, the faculty members of Department of Chemistry, delegates coming from different universities and colleges, my dear students, on behalf of Kharagpur College, I cordially welcome all of you to the one day International Seminar on "Emerging Trends in Science and Technology" organized by the Department of Chemistry of the College.

First and foremost, I express my thanks to the respected resource persons for spending their valuable time to make the event a successful one. All of them are very busy with their commendable academic and research activities. In spite of that, they have managed to come over here. I gladly acknowledge your contribution.

The department of Chemistry has been organizing seminars, webinars, special lectures, certificate courses and many other academic activities throughout the year. Their involvements in these activities are also reflected in their results. Results of Chemistry department are consistently good. Many alumni of the department are well placed in different jobs and research positions throughout the country and abroad. One such young alumnus, Dr. Milan Pramanik, who passed out from the college in the year 2017, is a speaker of today's seminar. We are proud of Dr. Pramanik and many such alumni who bring laurels to our college. Faculty of Chemistry of our college is also very rich comprising ten dedicated teachers with a balanced mixture of youth and experience. Teachers of the department are also carrying good quality research. Dr. Indranil Chakraborty was enlisted in the world ranking of top 2 % scientists Published by Stanford University in 2021. I hope that other faculty members will also receive awards and recognitions for their research works in near future.

Science and technology share a close relationship where the technology is essentially the scientific knowledge to create practical solutions and devices that interact in a common interface. From the very beginning of human civilization, humans have been finding solutions of the problems faced for the sake of their survival. In doing so innumerable technologies have been invented that have prospered civilization. We are still in search of new technologies.



The very day when primitive human beings discovered fire, a very important milestone was set up. Fire changes human life and its discovery might be considered as the foundation for development of Science and Technology. The way early humans controlled and used fire for satisfying their own needs, undoubtedly laid the groundwork for early Physics and Chemistry that has led to the development of modern technology through discovery in energy materials and beyond.

Now we have entered an age where artificial intelligence has been playing a very important and transformative role in the development of Science and Technology. AI is not just a tool but a catalyst for scientific and technological development. It speeds up discoveries, opens up new frontiers and reshapes how we understand and interact with the world. Its impact in enhancement of research and innovation in the areas of biology, medicine, physics and astronomy, driving technological advancement in robotics and material science is worthy of mention. It has bridged interdisciplinary studies which include but are not limited to bioinformatics, computer science, environmental science etc. However, in today's perspective, it's immensely essential to guide its development with ethical considerations and inclusive global cooperation, so that it can only be used for the upliftment and well being of human civilization.

Today's seminar is specially meant for making the students of our college and some nearby colleges and university, to acquaint with basic understanding of the recent scientific advancements and technological development. That will also motivate them towards research. Students and faculty members from different academic and research institution of the state and beyond have also joined the seminar. Thanks to the organizers for not restricting the scope of the seminar to narrow based area so as to create an opportunity to participate from all branches of academia. The current seminar would therefore, be a golden opportunity for the students for being exposed to the modern scientific investigations and technological developments through interactions with experts in the diverse focused field of the seminar. I am sure that the insightful deliberations and interactions of the students with the eminent teachers/scientists of the field will definitely help them develop curiosity and interest in the subject. The faculty members and research scholars will definitely be greatly benefited out of this seminar.

I presume that, today's seminar will give rise to some multidimensional pioneering contemplation that might lead to further development in the area of science and technology.

I wish all round success of the seminar. Thank you all. Have a good day.



Dr. Bidyut Samanta Principal, Kharagpur College

&

Chairman, Seminar Organising Committee



### Organizing Secretary's words

It gives me immense pleasure to welcome you all to this seminar on "Emerging Trends in Science and Technology" organized by the department of Chemistry, Kharagpur College on 23<sup>rd</sup> May 2025.

As the Organizing Secretary, it is both an honor and a privilege to say a few words about the seminar, as well as the department.

The department started its journey in the year 1972, and the honours subject was introduced in the year 1997. Currently we have 10 full-time faculty members. Over the years, the department has produced a large number of quality students, most of them are well established in different government and private sectors. Many of our recent students are currently pursuing their Ph.D./Post-doc in USA, UK, Japan, Germany and other places. This kind of seminar is a key part of our success in producing quality students, motivating them for higher education, as well as to enrich ourselves. Additionally, the department also arranges industrial visits or tours to higher academic institutes to keep the students updated with the advancement of science and technologies and for inspiring them.

This seminar is a platform where brilliant minds meet, amazing ideas flow, and high-tech innovation takes shape. In an age where technology is evolving faster than ever, staying informed and adaptable is no longer a choice — it's a necessity. From artificial intelligence and quantum computing to green energy and biotechnology, the scope of advancement is vast and growing every day. Today we have our speakers who will shed light on emerging trends in structural biology, chemistry of sulfur in pharma industry and technology development, and other aspects of current science and technology developments.

Our goal with this seminar is to shed light on these developments, provoke thoughts, and encourage collaboration. We are proud to host a lineup of distinguished experts, both national and international, who will share their insights, experiences, and predictions about what lies ahead.

Last but not least, this event would not have been possible without the tireless efforts of our dedicated team and the generous support of our institution. I sincerely thank each one of you for your cooperation and support.

Let us use today, not only to learn but also to connect — to ask questions, to share, and to spark new ideas that may very well lead to the next big breakthrough.

Once again, I welcome you all, and I hope this seminar proves to be insightful, engaging, and inspiring.

Thank you.

Mrs. Kuheli Pramanik Head, Department of Chemistry Secretary, Seminar Organizing committee



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# Key Note Address



### KN

### New Trends in Structural Biology

#### **Prof. Amit Kumar Das**

Department of Bioscience and Biotechnology IIT Kharagpur, West Bengal

To understand the structures is always an interesting topic to discuss. To begin with, Andreas Vesalius in 1543 wrote a book De Humani Corpis Fabrica, that marked a revolution in our understanding of the structure of the human body. Similarly, structures of high raising buildings, towers, bridges, tunnels, aero crafts etc. attract interest from common people to specialists in the field and their dimensions are in visible range. But, biologists and chemists are interested to know the structures of molecules and atomic resolutions (in Angstrom) that deciphers almost accurate bond lengths and bond angles to define the stereochemistry of the molecules. The variations of the stereochemistry deliver different functions of the molecules. microscopy can reach to a resolution that shows the existence of an entire universe of organisms all too small to be seen with the naked eye. When the first atomic structures of salt crystals were determined by the Braggs in 1912–1913, the analytical power of X-ray crystallography was immediately evident. Structural biology deals with the determination of the three dimensional structures of biological macromolecules (protein, DNA) at atomic resolution, and the use of those structures to explain the biological properties of those molecules in chemical terms. The triumph in structural biology was the structure of DNA that was published by Watson and Crick in 1953. Further, the structure of myoglobin (in 1960) that binds molecular oxygen reversibly, and lysozyme (1965) that hydrolyses polysaccharides are the beginning of structural biology to chemical understanding of molecular function. Time and again structural biology has been recognized as possessing great explanatory power, giving us visions of the atomic details of biological macromolecules that provide deep insights into how they are synthesized and fold, how they bend and flex, and how they interact with one another in performing their cellular and extra-cellular duties. All these structures were solved using single crystal x-ray crystallography technique. The bottlenecks for determining the structures using x-ray crystallography are (i) to purify homogeneously in large quantity (in milligram level), (ii) to crystallize such a large molecule, (iii) to get a high resolution diffraction data, (iv) to determine the phases of the reflections, (iv) to achieve the high quality computational facility, (v) to achieve cryo cooling technology and (vi) to gain high intensity x-ray and fast data collection. Further to these techniques, it requires high brilliance x-ray range using either sealed tube, rotating anode x-ray generator or synchrotron facility. Though theoretically, any size of the macromolecules should provide the high resolution diffraction, but it is very difficult to attain because of the stability of macromolecules are short lived. The problem of solving the large assembly of macromolecules, say virus, ribosome, is overcome by the new technique, the single particle cryo-electron microscopy / tomography. With time, the number of macromolecular structures has been



increasing, and now-a-day, with the use of artificial intelligence and deep learning, the structure of macromolecules or assemblies can be predicted. All these advancements have progressed our knowledge for drug or therapeutic designing for the human benefits. Structural biology is also at the heart of drug development and underpins the design of proteins with novel functions and even of new biomaterials. The day has long past when so little was known about macromolecular structure. We are still some way short of having a complete view of what has been called the 'molecular sociology' of life. We can marvel at the sophisticated molecular machinery within us but still feel unconnected - this is not how we usually see ourselves. Human as machine is very much the story being told or illustrated in science fiction by structural biology.



# Invited Lectures



### IL-1

# Regioselective C-H Activation: A Strategic Approach to Functionalized Arenes and Aldehydes

### Subhash Chandra Ghosh

GSC Lab, Marine Natural Products and Bio Polymers Division, CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar, Gujarat e-mail: scghosh@csmcri.res.in; schandra1976@gmail.com

**Abstract:** C-C and C-N bond formation are fundamental transformations in organic synthesis, underpinning the creation of diverse molecules with applications in pharmaceuticals, natural products, agrochemicals, and materials. Traditionally, these bonds have been formed through functional group interconversions or transition metal-catalyzed cross-coupling reactions, often requiring pre-functionalized starting materials and generating significant waste. Direct C-H bond functionalization offers a more atom-economical and sustainable alternative, minimizing waste generation. However, achieving selective C-H bond functionalization within complex molecules remains a significant challenge. Directed C-H activation strategies address this challenge by employing directing groups to guide the catalyst towards the desired C-H bond, enabling site-selective bond formation.

Figure: Strategies of regioselective C-H activation & functionalization of naphthalene



Our research group has developed a diverse array of catalytic systems for the regioselective functionalization of arenes and heteroarenes, encompassing reactions such as carboxylation, amination, amidation, etherification, alkylation, and annulation.<sup>[1]</sup>

Recently, we have successfully developed a novel Pd-catalyzed strategy for the direct C-H arylation and amidation of quinoline-8-carbaldehydes, enabled by chelation-assisted C-H bond activation.<sup>[2]</sup>

Furthermore, we have successfully applied these developed methodologies to the synthesis of important pharmaceutical compounds.

#### **References & Notes:**

1. (a) S. Sarkar, T. Sahoo, C. Sen, S. C. Ghosh *Chem. Commun.* **2021**, *57*, 8949–8952; (b) H. Singh, C. Sen, E. Suresh, A. B. Panda, S. C. Ghosh *J. Org. Chem.* **2021**, *86*, 3261–3275; (c) C. Sen, B. Sarvaiya, S. Sarkar, S. C. Ghosh *J. Org. Chem.* **2020**, *85*, 15287–15304; (d) C. Sen, T. Sahoo, H. Singh, E. Suresh, S. C. Ghosh *J. Org. Chem.* **2019**, *84*, 9869–9896; (e) N. B. Rathod, R. N. Patel, S. D. Patel, D. M. Patel, M. A. Sonawane, D. G. Thakur, S. C. Ghosh *J. Org. Chem.* **2024**, *89*, 18436–18444.

2. (a) D. G. Thakur, T. Sahoo, C. Sen, N. Rathod, S. C. Ghosh *J. Org. Chem.* **2022**, *87*,16343–16350; (b) D. G. Thakur, N. B. Rathod, S. D. Patel, D. M. Patel, R. N. Patel, M. A. Sonawane, S. C. Ghosh *J. Org. Chem.* **2024**, *89*, 1058–1063; (c) D. G. Thakur, M. A. Sonawane, R. N. Patel, N. B. Rathod, S. D. Patel, D. M. Patel, S. C. Ghosh *Adv. Synth. Catal.* **2024**, *366*, 4994–5000.



### IL-2

# From Bonds to Benefits: Sulfur-Containing Molecules in Organic Synthesis and Technology

### Milan Pramanik

Postdoctoral Research Associate, School of Chemistry, Cardiff University, United Kingdom

Abstract: Sulfur is a vital element with multifaceted roles across biological systems, pharmaceuticals, and modern technology. Its unique chemical versatility enables the construction of diverse molecular architectures, making sulfur-containing compounds indispensable in medicinal chemistry, materials science, and catalysis. In this talk, titled "From Bonds to Benefits," I will present our strategic approaches for the synthesis of value-added sulfur-based molecules with relevance to both the pharmaceutical industry and emerging technologies. The core focus will be on innovative synthetic methodologies involving iodine reagents, non-covalent interactions, photocatalysis, borane catalysis, and Frustrated Lewis Pair (FLP) chemistry. These approaches enable selective and efficient formation of C-S bonds, which are central to the design of biologically and industrially significant molecules. Key transformations to be discussed include hydrothiolation, sulfonylation, modified Knoevenagel condensation, and cascade chalcogenation strategies, all contributing to the enrichment of sulfur-containing scaffolds. Additionally, I will address the capture and chemical utilization of carbon dioxide (CO<sub>2</sub>) — a critical challenge in the context of global sustainability. Our work demonstrates how sulfurbased reactivity platforms can contribute to CO2 conversion, offering a pathway toward greener and more sustainable chemical technologies.

This talk will highlight the journey from fundamental bond-forming strategies to real-world benefits, showcasing sulfur's enduring impact on the future of chemical science



### IL-3

### Magneto Impedance Effect in Electrodeposited Wires for Sensor Applications

### **Amaresh Chandra Mishra**

Assistant Professor, Department of Natural Sciences, PDPM Indian Institute of Information Technology, Design and Manufacturing ,Jabalpur

Magnetoimpedance (MI) effect, is a phenomenon observed in soft magnetic materials where the electrical impedance of the material can be altered as a function of external magnetic field. It works on the basic mechanism of tuning of skin depth which can be achieved through change of transverse permeability under the influence of magnetic field. Cylindrical wire geometries are preferred candidate for MI owing to high degree of symmetry and thus negligible demagnetization effect in circumferential direction. A soft magnetic film coated over a nonmagnetic wire exhibits higher MI effect in terms of quantitative change as compared a solid ferromagnetic wire. Thus, such samples are paid more attention in recent past. These composite film coated wires are prepared by electrodeposition. The composition and pH of the bath, current density during electrodeposition and organic additives present in bath influence the MI performance of the deposited wire.



## Oral Presentation



# Electrochemical Water Oxidation Catalysis by 1st row Transition Metal Complexes

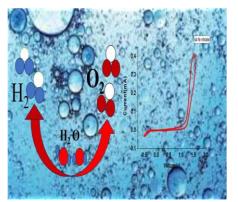
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**Abstract**: Water electrolysis is among the simplest method for generating hydrogen as an alternative renewable fuel. A major challenge associated with this process is the development of cheap, simple and environmentally benign catalysts for water oxidation that lead to a minimum over potential. Within this process, the oxidation of water into molecular oxygen is considered as the bottleneck reaction because it involves the transfer of four electrons toward the oxidation of a highly stable small molecule. Challenges in this area include the development of stable and effective electro- and photocatalysts that utilize readily available metal ions. Herein we report a copper-peptidomimetic complex as an electrocatalyst for water oxidation, which is both highly stable and efficient. Inspired by enzymatic catalysis, which is largely based on intramolecular cooperativity between a metal centre and functional organic molecules located on one scaffold, we have designed and synthesized a peptoid trimer bearing a 2,2'-bipyridine (bipy) ligand, an -OH group, and a benzyl group. Another way inspired by the Mn4CaOx cluster that catalyzes water oxidation in photosystem II, described here is the synthesis and characterization of the manganese cluster [Mn<sub>12</sub>O<sub>12</sub>(O<sub>2</sub>CC<sub>6</sub>H<sub>2</sub>(OH)<sub>3</sub>)16(H<sub>2</sub>O)<sub>4</sub>] (Mn<sub>12</sub>TH) along with its electrocatalytic activity at pH 6. Electrochemical, spectroscopic, and electron microscopy studies show that Mn<sub>12</sub>TH is a homogeneous electrocatalyst for water oxidation and enables oxygen evolution



with a reaction rate of 22s<sup>-1</sup>, high Faradic efficiency (93%), and an overpotential of only 74 mV, the lowest reported to date.

*Keywords:* metal complex, electrolysis, water oxidation, renewable energy, overpotential

**References:** (1) Ghosh *et.al.* **ACS Catal.2018**, 8, 10631–10640.(2) Ghosh *et.al.* **Angew. Chem. Int. Ed. 2019**, 58, 2785–2790. (3) Ghosh *et.al.* **Angew. Chem. Int. Ed. 2018**, 130 (26), 7829-7834.(4)*karim et.al.* **Catalysis Science & Technology, 2020**, 10 (9), 2830-2837.



# Antiviral Activity of Boswellia serrata Resin Extract Against HSV-1 Through Modulation of NF-κB Pathway

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Abstract: Although *Boswellia serrata* gum-resin is traditionally used for managing skin disorders, its antiviral potential against HSV-1 remains underexplored. This study investigates the antiviral efficacy and mechanism of action of the methanolic extract of *B. serrata* resin (BSR) against HSV-1. The extract underwent standard extraction, fractionation, and standardization protocols. Cytotoxicity (CC<sub>50</sub>) and antiviral activity (EC<sub>50</sub>) were assessed using MTT and plaque reduction assays. A time-of-addition assay, supported by RT-PCR, determined the temporal efficacy of BSR, while RT-PCR was also employed to measure expression levels of key immunomodulatory markers. BSR exhibited potent antiviral effects against both wild-type and clinical HSV-1 strains, achieving near-complete inhibition (EC<sub>99</sub>) at 10 μg/ml, particularly when administered 1 hour post-infection. The extract downregulated NF-κB and p38 MAP kinase activity and significantly reduced the expression of pro-inflammatory cytokines TNF-α, IL-1β, and IL-6. These results support the ethnomedicinal use of *B. serrata* and highlight its therapeutic potential against HSV-1 by targeting the NF-κB signaling pathway.

**Keywords:** NF-κB, Cytotoxicity (CC<sub>50</sub>), *Boswellia serrata*.



# Synthesis of Azepinoindolone Derivative using Larock's Heteroannulation and Lactamization

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**Abstract**: Paullones are the series of fused tetracyclic compounds containing the indolo[3,2-d][1]benzazepin-6(5H)-one structure. They have been described as potent, ATP-competitive inhibitors of the cell cycles regulating cyclin-dependent kinases (CDKs), glycogen-synthase kinases (GSKs) and mitochondrial malate dehydrogenase (mMDH) and have become a class of very useful agents for the treatment of neurodegenerative and proliferative disorders. Thus, indoles containing seven-membered lactum rings have been isolated from several natural sources and form a significant series of medicinal agents.  $^1$ 

Here, a synthetic route for 3,4,5,6-tetrahydroazepino[4,5-*b*]indol-2(1*H*)-one derivatives have devised using Larock's heteroannulation reaction as the key step.<sup>2</sup> The seven-membered lactum ring was synthesised from suitable 2,3-disubstituted indole and indole precursor formation took place *via* Larock's heteroannulation<sup>3</sup> by Pd(II) catalysis between internal alkyne and tosyl protected 2-iodoaniline. The internal alkyne was obtained by coupling between ethyl diazoacetate and protected homopropargyl alcohol following Greg Fu's method.<sup>4</sup>

#### **References:**

- 1. Cao, Z.; Zhu, J-B.; Wang, L.; Liao, S.; Tang, Y. Org. Lett. 2019, 21, 4097.
- 2. Chakraborty, A.; Ankita, Kumari, N. Kumar. R. Research Review International Journal of Multidisciplinary, 2023, 08, 52.
- 3. Larock, R. C.; Yum, E. K.; Refvik, M. D. J. Org. Chem. 1998, 63, 7652.
- 4. Suárez, A.; Fu, G. C. Angew. Chem. Int. Ed. 2004, 43, 3580.



# Modulating CO<sub>2</sub> reduction product selectivity with ligand environment around Cu-based molecular catalysts

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Abstract: Electro-catalytic CO<sub>2</sub> reduction to HCOOH offers a sustainable route for carbon capture and utilization, enabling renewable energy storage and producing a valuable chemical and hydrogen carrier under mild conditions. Few non-noble metal molecular catalysts are reported that facilitate the electrocatalytic reduction of carbon dioxide to Formic Acid. Here, we have synthesized a series of Cu-based molecular catalysts, string from redox active bipyridine & pyridyl-triazole ligand system co-ordinate with Cu centre form C1: Cu(bpy)<sub>2</sub>, C2: Cu(pyridyltriazole)<sub>2</sub>&C3: Cu(bpy)<sub>2</sub>(pyridyl-triazole)<sub>2</sub> for electrochemical reduction of CO<sub>2</sub>. Cu(bpy)<sub>2</sub> and Cu(pyridyl-triazole)<sub>2</sub> exclusively reduced CO<sub>2</sub> to CO with TON of 177 and 183, respectively. Interestingly, by modulating the electronic environment and molecular geometry around the copper(II) center of the C3 catalyst via heteroleptic ligation, we can effectively tune the product selectivity in the electrochemical CO<sub>2</sub>RR from carbon monoxide (CO) to formic acid (HCOOH). In this work, we report the first example of a molecular copper-based active center, Cu(bpy)<sub>2</sub>(pyridyl-triazole)<sub>2</sub>, that demonstrates selective electrochemical conversion of CO<sub>2</sub> to HCOOH, achieving a turnover number (TON) of 197. Owing to their remarkable catalytic activity, these systems have garnered considerable research interest, particularly due to their potential for scalable applications. To further assess their practical viability, we investigated their performance under heterogeneous catalytic conditions. In this context, we synthesized heterogeneous Cu-based functionalized materials, namely C2@GO and C3@GO, through amide bond formation between the free amine (-NH<sub>2</sub>) groups and graphene oxide (GO) from the molecular catalysts C2 and C3, respectively. The resulting hybrid materials, C2@GO and C3@GO, exhibited selective electrocatalytic reduction of CO<sub>2</sub> in a CO<sub>2</sub>-saturated bicarbonate solution (pH 6.9), predominantly producing CO and HCOOH with faradaic efficiencies of 72% and 82%, respectively.



### Ethnomedicinal Survey of Monocotyledonous Plants in Belpahari, Jhargram District, West Bengal, India

### Happy Das

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Abstract: The study concerns the monocot plants in Belpahari, a beautiful area in West Bengal famous for its tribal people. Studies show that many elderly and health experts in the area use nearly 45 different monocots as medicines. All these plants are economically as well as ecologically important. Historically, folk medicine using medicinal plants focused on healing fever as well as illnesses affecting the digestive, lung and skin functions. Due to being anti-inflammatory and antibacterial, many people like these plants. It also describes using decoctions, poultices and infusions, along with the preferred rhizomes, leaves and stems from different herbal plants. Indigenous people possess valuable knowledge about the plants in their surroundings and we should try our best to protect this wisdom. The research increases understanding of ethnobotany and also encourages people to protect the plants and traditions of the area. Based on the research, many local traditions surround these plants, indicating they should be protected for the benefit of future generations. Based on this research, I think there is valuable information on rural Indian healthcare that relies on plants and currently includes aspects of local knowledge in medicine.

Keywords- Belpahari, Ethnobotany, Tribal people, Folk medicine



### Adsorption of Toxic Cd (II) Pollutants on a β-Cyclodextrin based Antibacterial Hydrogel Gel towards Fabrication of a Gel Electrolytebased Supercapacitor

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Abstract: Water and energy both are extremely crucial in this contemporaneous world. Therefore, advanced technologies intended at minimizing water pollution as well as creating sustainable energy storage systems are key areas of global research. Cadmium pollution poses a significant risk to human health. In response, a crosslinked β-CD based hydrogel has been developed by grafting and crosslinking poly(N-isopropylacrylamide) [pNIPAAm] and poly(2-Acrylamido-2-methylpropane sulfonic acid) [pAMPS] onto the backbone of β-CD. This hydrogel, which is biocompatible, biodegradable, and antibacterial demonstrates outstanding pH and temperature-sensitive Cd<sup>2+</sup> adsorption capabilities from wastewater. It efficiently removes most Cd<sup>2+</sup> from water, adhering to the Langmuir adsorption isotherm and following linear pseudo-second-order kinetics. Furthermore, the Cd<sup>2+</sup> loaded hydrogel has been repurposed as a gel electrolyte in a high-performance asymmetric supercapacitor for energy storage applications. When used in the construction of a supercapacitor, this hydrogel shows enhanced specific capacitance and energy density, achieving 203.84 A/g and 54.30 Wh/kg, respectively. The device remains highly stable and retains 77% of its charge even after 5000 cycles. Additionally, this gel-based supercapacitor can power both red and green LEDs.

**Keywords:** Hydrogels; Adsorption; Supercapacitors; Cadmium ions; Gel-electrolyte



# The influence of non-covalent interactions in metal-free organic dye molecules to augment the efficiency of dye sensitized solar cells: A computational study

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**Abstract**: The efficiency of dye sensitized solar cells (DSSCs) can be enhanced with achieving better planarity of metal-free organic dye molecules and thinning of their aggregation on the semiconductor surface.<sup>1,2</sup> We report that the subtle noncovalent N...S interaction between the substituted phosphazene group and thiophene spacer unit in dye molecule which induces the desired planarity and avoid aggregation of such molecules on the TiO2surface using DFT calculations. DFT results show that phosphazene group increases the maximum absorption wavelength ( $\lambda_{\text{max}}$ ), driving force for electrons injection ( $\Delta G_{\text{injection}}$ ), singlet excited state lifetime ( $\tau$ ), dipole moments ( $\mu_{\text{normal}}$ ), and number of electrons transferred from dye to TiO<sub>2</sub> surface ( $\Delta q$ ), which are known to augment the efficiency of DSSCs. Further, the lower  $\Delta G_{\text{regeneration}}$  value of phosphazene containing dyes (e.g., -.37 eV, dye 2) than the reported dyes (e.g., -.81 eV, dye 1) indicate the faster electron injection rate from the former dye to the semiconductor TiO2. The role of phosphazene group to prevent the aggregation of dye molecules on the TiO2 anatase surface was also examined with GGA-PBE/DNP level of theory. The calculated results suggest that the dye molecules on 1-(TiO<sub>2</sub>)<sub>38</sub> and 2-(TiO<sub>2</sub>)<sub>38</sub> anatase clusters avoids the aggregation due to the steric congestion induced by phosphazene group. This work reports to accomplish dual properties with subtle noncovalent interactions in dye molecules to augment the efficiency in DSSCs.

### **References:**

- 1. B. O' Regan and M. Gratzel, *Nature* **1991**, *353*, 737–740.
- 2. A. K Biswas, A, Das and B. Ganguly, International Journal of Quantum Chemistry, 2017, 117, 25415.



### Nanoclay-Filled TPE-Based Hybrid Nanocomposites: Design and Multi-Scale Characterization

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**Abstract:** The pursuit of polymeric materials with enhanced properties has recently driven increased interest in nanostructured fillers, which are key to develop high-performance polymer nanocomposites. The nanoparticles are used in immiscible polymer blends as compatibilizers. Of the various candidates for nanocomposite precursors, clay and layered silicates have received the most extensive research attention. This study aims at investigating the effects of pristine and modified laponite clay on a model thermoplastic elastomer (TPE) blend system composed of low-density polyethylene (LDPE) and ethylene vinyl acetate copolymer (EVA). Melt blending was employed to incorporate two distinct nanoclay particles into this system at 1.5 wt% loading. The clay particles were modified via ion exchange method to enhance their compatibility with the polymer matrix. The resulting blends were compression moulded and characterized for mechanical, dynamic mechanical, thermal properties, and morphology. The properties of the blends are found to be strong function of the extent of modification. An enhanced mechanical performance is consistently observed across all nanoclay-reinforced films. Morphological analyses and dynamic property measurements reveal that the variations in blend system properties mainly arise from the degree of nanofiller dispersion and changes in crystalline morphology, both of which strongly depend on the preferential localization within the LDPE or EVA phases and the propensity of the nanofillers to form aggregates.

**Keywords:** Blends, TPE, clay, dispersion, morphology, nanocomposites.



# Fluorescence Sensing of Metal ion: A Complete Study with newly synthesized Schiff Base ligand and Metal complex

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**Abstract**: Metal ion sensing is always very crucial from biological point of view. In search of new ligand for vital metal ion Zn 2+ sensing, a zinc coordinated rare binuclear complex was synthesised and characterized by elemental analyses and single-crystal X-ray diffraction. Two two mononuclear units formed Schiff base ligands 2-((2-(pyrimidin-2by yl)hydrazono)methyl)phenol (PHP) coordinated with zinc ion are bonded together through a hydrogen atom to form the binuclear complex. This phenomenon was investigated by several experimental procedures like UV-Vis absorption, fluorescence, proton NMR spectra and theoretical calculations to explain the response. PHP can selectively respond to Zn<sup>2+</sup>with the fluorescence "turn-on" owing to the formation of the complex in the solution. There also exist hydrogen bonding interactions and C-H··· $\pi$  interactions in the crystallographic structure of binuclear complex. Moreover, densityfunctional theory was employed for theoretical interpretation to validate the experimental outcomes and PHP-Zn<sup>2+</sup>complex formation. The receptor PHP successfully detect the Zn<sup>2+</sup> ion in PC-3 i.e. human prostate carcinoma cells by Confocal microscope.

**Keywords:** Sensing, complex, fluorescence, DFT, imaging.



### The role of technological innovation in England's Industrial Revolution

#### **Uttam Das**

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Abstract: Since the end of the middle Ages, the demand for manufactured goods increased due to the gradual increase in population, improvement in agriculture, per capita income, etc., and it became increasingly difficult for the former craftsman to keep up with the supply. In order to increase the efficiency of the craftsman, the merchant appeared in the field of production for the sake of his own profit. Attempts are made to meet the increased needs of the society by changing it through various experiments. Ultimately, centralization and ministerialization of the production system provides the full solution to the gap between demand and supply. The factories of the modern age were established with the destruction of the old cottage industry, where the capitalist owner found it profitable to rely on magic rather than manual labour. So in a limited sense, the rapid production of low-cost goods with the help of machinery can be termed the Industrial Revolution. At the same time, however, it should be remembered that 18. It should be noted that this industrial revolution of the 18th and 19th centuries had a far-reaching social and political 1 background and its far-reaching impact not only on the economy, but also on society, politics and even human consciousness. Therefore, while discussing the role of technology and science in the industrial revolution, one must be aware that various technological and scientific discoveries take place in a particular situation. This is easy to understand when we remember that human society has experienced many technological advances even in the truly modern era, but breakthroughs like the Industrial Revolution have never been possible before. So the bottom line is discussed exactly under which circumstances the discoveries could have an impact. Its background is more important to the historian than just technology and science. Innovation refers to scientific discoveries related to technology and their successful, commercial application in production technology. Innovation is therefore not strictly a scientific matter, rather it is a mixed result of psychology, sociology, economic dynamics etc. Technological innovation played an active role in Britain's Industrial Revolution. However, it is also true that it would not have been so effective if other pressures were not present. At the same time, the production would not have increased without the sudden increase in demand from various sectors, such as the domestic sector, the export sector, the government sector, resulting in an increase in the profit potential. Similarly, if production did not increase, investment would not increase, capital accumulation would not increase, commercial use of scientific discoveries would not be possible. Technological innovation is therefore a mixture of all.



# Double averaged turbulence properties in rough bed open channel flow: Theoretical Background

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**Abstract:** The three-dimensional heterogeneous flow over the roughened bed plays a significant role in fluvial geomorphology. This article deals with the problem of understanding the turbulence flow properties over various roughned beds. The time-averaged (TA) turbulence properties are unable to predict the accurate result about the understanding of the threedimensional flow phenomenon for specific flow zones over different kinds of bottom roughness. Moreover, the present study particularly focuses on the changes in double-averaged (time and space) turbulence characteristics governed by the double-averaged (DA) Navier-Stokes equations. This article proposes the momentum equations of wave-current flow on various kinds of roughened beds. Moreover, the mechanisms behind changes in DA turbulence flow properties, focusing on both natural rough beds and artificial rough beds (both permeable and impermeable), are controlled in laboratory flume experiments. These equations highlight the changes in DA turbulence parameters that influence the roughness elements and assess the usefulness of various turbulence properties for describing three-dimensional wave-current flow physics in different flow layers owing to the flow-roughness interaction. Therefore, a clear understanding of such flows over the hydraulically rough bed (Fig. 1.1) is needed for accurate modelling of sediment entrainment and coastal protection. The geometry of the various types of the natural occurrence of rough beds in open channel flow controls the turbulent flow characteristics of the near-bed region. It plays a key role in the near-bed mass and energy transfer with the outer flow. In environmental hydraulics, the characteristics of the turbulent flow over and within the rough bed serve as the identification of the flow layers, flow types, flow resistance, transport of suspended sediments, and flow-biota interaction. Therefore, the quantification and understanding of the physics of the rough bed turbulent flow attracted the attention of researchers and scientists in several disciplines, such as environmental hydraulics, geomorphology, earth science, engineering, as well as physics and applied mathematics.



Fig. 1.1. Various kinds of natural rough bed

**Keywords:** Double-average; Turbulence intensity; Form-induced intensity; Reynolds stress; Form-induced stress; Turbulent kinetic energy; Turbulent kinetic energy budget; Anisotropy; Roughness layer; Outer layer.



# Self-assembly of sodium and potassium betulinates into gels and synthesis of gel-gold nanoparticle hybrid materials

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**Abstract:** Study of the self-assembly of small molecules in different liquids via non-covalent forces yielding gels has become a rapidly expanding area of research because the supramolecular gels thus obtained have various potential and realized applications.[1] Self-assembly of molecules yielding hydrogels is of special signficance due to their range of applications in drug delivery, tissue engineering, cosmetics, removal of toxic chemicals, etc.[2] Betulinic acid 1 is a nano-sized pentacyclic monohydroxy triterpenic acid extractable from the barks of *Ziziphus jujube* (Z. jujube), *Betula papyrifera* (white birch), etc. having tremendous medicinal signficance as anticancer, antitumor, antidiabetic and anti-HIV activities. Excellent gelation ability of betulinic acid in different liquids via the formation of fibrillar networks has been reported earlier.[3] Currently, the self-assembly properties of sodium and potassium salts of betulinic acid 2 and 3 respectively in water as well as aqueous solvent mixtures along with the morphological characteristics of the self-assemblies has been explored.[4] Both the salts spontaneously self-assembled into fibers of nano to micrometer diameters yielding supramolecular gels. The



hydrogels of sodium and potassium betulinates have been utilized for entrapment and removal of toxic dye such as rhodamine-B (rho-B). Synthesis of gel—gold nanoparticle hybrid materials by utilizing the hydrogels of both sodium and potassium betulinates and in situ generated gold nanoparticles, obtained by the reduction of Au(III) with the bark extract of Z. jujube have also been demonstrated at room temperature (Fig. 1).

**Fig. 1:** Schematic representation of self-assembly of salt of betulinic acid into hydrogels.

**References:** [1] B. G. Bag, S. S. Dash, *Langmuir*, **2015**, 13664-13672. [2] M. Suzuki and K. Hanabusa, *Chem. Soc. Rev.* **2009**, 38, 967–975. [3] B. G. Bag, S. S. Dash, *Nanoscale*, **2011**, 3, 4564–4566. [4] B. G. Bag, S. S. Dash, *RSC Advances*, **2016**, 17290-17296.



### Synthesis of Reduced Pyranonaphthoquinone and Its Aza-analogue Using Palladium Catalyst

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**Abstract:** Pyranonaphthoquinones, which are prevalent in nature, constitute an important research area in organic synthesis due to the pronounced biological activities of these heterocyclic compounds.<sup>1</sup> The pyranonaphthoquinone antibiotics<sup>2</sup> have been isolated from various strains of bacteria and fungi of microbial origin and are typified by the presence of a basic naphtho[2,3-c]pyran-5,10-dione skeleton.

Their applicability for both biochemical and pharmacological use explains the synthetic efforts made by different chemists over the years.<sup>3</sup> In connection with our interest in palladium-mediated formation of heterocyclic molecules, the synthesis of reduced pyranonaphthoquinone and 2-Aza analogues of pyranonaphthoquinones via palladium(0)-catalyzed cyclization was envisaged.<sup>4</sup>

Figure 1: Synthesized reduced pyranonaphthoquinone and 2-Aza analogues

### **References:**

- 1. (a) Arsenault, G. P. *Tetrahedron Lett.* **1965**, 45, 4033–4037 and references therein; (b) Parisot, D.; Devys, M.; Barbier, M. *J. Antibiot.* **1989**, 42, 1189–1190.
- 2. Brimble, M. A.; Duncalf, L. J.; Nairn, M. R. Nat. Prod. Rep. 16, 267 (1999).
- 3. Croisy-Delsey, M.; Carrez, D.; Bisagni, E. Eur. J. Med. Chem. 1988, 23, 101-106.
- **4.** (a) Nandi, S.; Samanta, S.; Jana, S.; Ray, J. K. *Tetrahedron Lett.* **2010**, *51*, 5294, (b) Nicolaou, K. C.; Li, H.; Nold, A. L.; Pappo, D.; Lenzen, A. *J. Am. Chem. Soc.* **2007**, *129*, 10356.



### Advancement towards the development of metal organic framework for the detection of organic pollutants

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Abstract: The presence of organic pollutants beyond its normal limit poses serious threats to public health and ecological balance. Exposure to toxic chemicals in the environment can lead to serious health problems, such as cancer and respiratory conditions like asthma. Several types of organic pollutants exist, including pesticides, dioxins, volatile organic compounds, polychlorinated biphenyls, and various hydrocarbons. Designing sensing probes that can selectively and sensitively detect specific organic pollutants are necessary for environmental monitoring and public health protection. In the field of sensing, MOFs have shown great promise for the detection of various organic pollutants, including pesticides and volatile organic compounds. The properties of MOFs, including tunable porosity and high surface area, make them well-suited for sensing applications, particularly for detecting dioxins and other organic pollutants. Recent advances in MOF-based sensing technologies for dioxins and dioxin-like organic pollutants will be comprehensively presented.

**Keyword:** Metal organic framework, Organic pollutants, Dioxin, Pesticides, Aromatic hydrocarbons, Polyaromatic hydrocarbons

#### Reference:

1. Banshidhar, S. Paladhi, K. Shah\*, L. Singh\* Chemosphere, 2025, 379, 144428.



# Chemically Grown Nickel Oxide Nanoparticles for Photodegradation of MB dye

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Abstract: In this study, Nickel Oxide (NiO) nanoparticles were synthesized using a simple and efficient chemical method. The structural characteristics of the sample were examined through X-ray powder diffraction (XRD), High-Resolution Transmission Electron Microscopy (HRTEM), while optical properties were analysed using UV-Vis absorption spectroscopy and Photoluminescence (PL). XRD analysis confirmed that the nanoparticles exhibited a face-centered cubic (FCC) structure. Transmission electron microscopy (TEM) revealed an average particle size of ~20 nm, and HRTEM further validated the crystallinity observed in XRD analysis. UV-Vis spectroscopy determined that the optical band gap of the nanoparticles was found to be in 4.48 eV. PL analysis suggested that the observed emission resulted from transitions involving defect states. The photocatalytic activity of NiO nanoparticles was investigated in the degradation of methylene blue (a cationic dye) under visible light irradiation. The degradation efficiencies were found to be 59% for methylene blue after one hour of illumination.

**Keywords**: Chemical precipitation; FCC; optical band gap; Photocatalytic activity; degradation efficiency.



### OP-16

### Advancement of Artificial Intelligence and its impact on Employment Pranim Rai

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**Abstract:** The world is witnessing rapid advancement of Artificial Intelligence (AI). AI is continually evolving and is progressively integrating into diverse aspects of modern economies—from manufacturing and healthcare to finance and education. While AI promises to increase efficiency, improve decision-making, and reduce costs, it also poses significant challenges related to job displacement, skill obsolescence, and economic inequality.

The fear that machines will displace human labour is not new. But the difference this time is that AI can perform not only physical tasks but also cognitive functions, putting a wider range of jobs at risk. AI is affecting sectors unevenly. Routine and repetitive jobs—both manual and cognitive—are the most susceptible to automation. On the other hand, sectors that rely on creativity, emotional intelligence, and complex decision-making—such as healthcare, education, and arts—are less likely to be fully automated in the near term. But possibilities of AI is such that it can infringe into these sectors as well.

AI's impact on employment depends on many factors, like the pace of technological adoption, responsiveness of education systems, and effectiveness of policy interventions. Ethically, there is a growing need to ensure that AI deployment enhances, rather than undermines, human well-being and dignity.

This paper explores the multifaceted impact of AI on jobs, examining how automation, machine learning, and intelligent systems are reshaping work across industries. It also evaluates policy responses and strategic approaches for workforce adaptation, including reskilling, lifelong learning, and inclusive innovation.



### OP-17

# Science as Story: Ethical Futures and Speculative Reason in Kim Stanley Robinson's *Novel*2312

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**Abstract:** Kim Stanley Robinson's 2312 presents a visionary setting that exemplifies the intersection of science and literature, using speculative fiction as a platform to explore humanity's future across a transformed solar system. Set in the year 2312, the novel features a meticulously detailed universe shaped by terraforming (a process of transforming planets and moons to be habitable by humans), space colonization, climate crisis recovery, artificial intelligence, and posthuman biology. This scientifically grounded world-building serves not only as a speculative projection of current technologies but also as a narrative device through which Swan Er Hong, the protagonist who is the artist from Mercury and a former "world designer" in Robinson's novel, examines philosophical, ecological, and socio-political concerns during that period.

The novel's setting functions as both context and commentary — an active participant in the story's exploration of what it means to be human in a time of radical climatic change. 2312 blurs the boundary between empirical inquiry and imaginative speculation, demonstrating literature's capacity to engage with scientific thought while offering critical perspectives on its application. Through its intricate setting, the novel acts as both a mirror of contemporary anxieties and a blueprint for future possibilities like terraforming, encouraging interdisciplinary dialogue and ethical reflection. This paper, thus, affirms the vital role of literature in envisioningthe trajectory of scientific and cultural evolution by enquiring in details the setting of 2312.

**Keywords:** Science fiction, speculative fiction, science and literature, interdisciplinary narrative, posthumanism, terraforming.



Poster Presentation

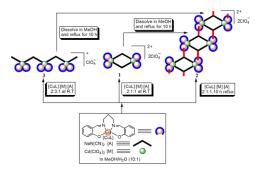


Supramolecular isomers based on a hetero-trimetallic Cu<sub>2</sub>Cd node and dicyanamide spacer in a hexanuclear cluster, a 1D stair polymer and a 1D zigzag chain

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**Abstract:** The synthesis and characterization of Coordination Polymer (CP) by using facile strategies has become a popular research topic in the field of supramolecular chemistry [1]. Robson formulated and illustrated one of the most powerful synthetic strategies for the construction of a large variety of coordination polymers: the node-and-spacer approach [2]. hetero-metallic Three copper(II)-cadmium(II) complexes  $[{(CuL)_2Cd}_2(\mu_{1.5} N(CN)_2)_2[(ClO_4)_2\cdot(H_2O)_2 (1),\{[\{(CuL)_2Cd\}_2(\mu_{1,3,5}-N(CN)_2)_2](ClO_4)_2\}_n$  (2) and  $\{[(CuL)_2Cd(\mu_{1,5}-H_2O)_2,H_2O)_2\}_n$ N(CN)<sub>2</sub>)](ClO<sub>4</sub>)<sub>n</sub> (3)have been synthesized using a trinuclear hetero-metallic node,  $[(CuL)_2Cd]^{2+}$  (where  $H_2L = N,N'$ -bis(salicylidene)-1,3-propanediamine) and dicyanamido spacer by varying the ratiosof the reactants and temperature. Complex 1 is a discrete hexanuclear cluster where two trinuclear nodes are connected through the Cd centres by convergent double  $\mu_{1.5}$ dicyanamido spacers. Complex 2 is a 1D stair coordination polymer in which the hexanuclear units are joined by the coordination of the central nitrogen atom of  $\mu_{1,3,5}$ -dicyanamido ligand to the Cu atom of another unit. In contrast, complex 3 is a 1D zig zag chain, formed by connecting the Cd centre of trinuclear nodes via divergent μ<sub>-1.5</sub>-dicyanamido spacers. These three complexes contain a common [(CuL)<sub>2</sub>Cd(N(CN)<sub>2</sub>)]ClO<sub>4</sub> trinuclear unit as molecular building block. They represent an example of "supramolecular isomerism" of 0D/1D coordination polymers.



#### References:

- [1] S.W. Jaros, J. Król, B. Bażanów, D. Poradowski, A. Chrószcz, D.S. Nesterov, A.M. Kirillov, P. Smoleński, Molecules 25 (2020) 2119–2132.
- [2] B. F. Hoskins, R. Robson, J. Am. Chem. Soc. 112 (1990) 1546–1554.



# Spectral studies on the interaction of Catatonic dyes with silica nanoparticles

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Abstract: This work focuses on the absorption spectroscopic study for the interaction of methylene blue and nano-colloidal dispersion of silica. Interactions are governed by electrostatic interactions and hydrophobic interactions, which influence the spectral characteristics of the dye. The binding constant and stoichiometry of dye-nanoparticle aggregates were determined by analysing the absorption spectra in presence of different silica concentration. From the shifts in the absorption peak (bathochromic shift), it was revealed some changes in the dye's electronic environment, i.e. electrostatic attraction between the cationic dye and negatively charged silica surface. Absorption spectral behaviour of methyelene blue and acridine orange were investigated to perceive the nature and extent of interaction with anionic silica nanoparticles.  $0.5 \times 10^{-5}$  M aqueous solution of methyelene blue and 2×10<sup>-5</sup> M acridine orange the visible absorption were recorded in the range 800-200 nm. Aqueous solution of Methyelene blue and Acridine Orange exhibits a band at 663 nm and 492 nm of the said concentrations. The spectral data with a fixed concentration of methylene blue and acridine orange and varying concentrations of the silica nanoparticles were suitably processed in determining the interaction constant between the dye and the polymers. For silica-dye aggregates, binding constant values were derived using the Benesi-Hildebrand formalism. Further investigations on the different formulations towards complete entrapment of dye molecules are under consideration.



### The Oyster Collection Algorithms

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Abstract: This article draws inspiration from one of nature's fascinating processes—the collection of oysters from the sea bed—to develop a novel class of metaheuristic algorithms. For living oysters, they are generally found in the cold-water region, but for non-living shells, they can be found anywhere in the sea bed, depending on the blow of the wind and the path of the water wave. These shells hold more than just ecological significance—they are highly valued for their use in decorative art, ornaments, and gift items, making oyster collection an important livelihood for many coastal communities. Inspiring from the nature of the collection procedure of the shells, we construct mathematical functions of the search path along which it can be available more. Utilizing this procedure into the field of optimization, we have found some noble results of a benchmark problem. Basically, we fit an appropriate test function for a benchmark problem, then some numeric experimental results are computed via oyster collection algorithms. A comparative study has also been made to validate the proposed approach. Moreover, the graphical illustrations show the efficacy of the proposed algorithms and, finally, a conclusion is made about keeping some scope for future works.

**Keywords:** Sea shell, Archimedean spiral, Search method, Metaheuristic algorithm, Optimization

**References:**[1] Meraihi, Y., Gabis, A.B., Mirajalili, S., Grasshopper Optimization Algorithm: Theory variants and Applications. **2021**.IEEE Access <a href="https://doi.org/10.1109/ACCESS.2021.3067597">https://doi.org/10.1109/ACCESS.2021.3067597</a>.

- [2] Johari, N.F., Zain, A.M., Mustaffa, N., Udin, A., Firefly Algorithm for Optimization Problem. Applied Mechanics and Materials. 2013. https://doi.org/10.4028/www.scientific.net/AMM.421.512.
- [3] Gandomi, A. H., Yang, X. S., Alavi, A. H., Mixed variable structural optimization using fire fly algorithm. Comput Struct. **2011**, 89 (23–24), 2325–2336.
- [4] Msadeh, R.M.T., Mahafzah, B.A., Aziz Sharieh, A.A., Sea Lion Optimization Algorithm. *International Journal of Advanced Computer Science and Applications***2019**, 10(5), 388-395. https://doi.org/10.14569/IJACSA.2019.0100548.
- [5] Kermany, S.D., **2020**. Tiger Algorithm, Conference: 2020 International Conference on High Performance Big Data and IntelligentSystems (HPBD&IS), https://doi.org/10.1109/HPBDIS49115.2020.9130593.



## Application of GIS Tools for Urban Sprawl Analysis and Prediction of Future Expansion in Kharagpur City, India

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**Abstract:** Urban sprawl refers to the rapid expansion of urban areas characterized by unplanned, unregulated, and uncoordinated expansion. Consequently, for urban planning that exceeds conventional boundaries, the direction and assessment of urban growth are essential. The objective of the present study is to assess the unique and temporal patterns of urban expansion regarding both magnitude and direction. This study incorporates Shannon's entropy model, the Normalized Difference Built-up Index, and the CA Markov Model to analyze current and future trends and patterns of urban sprawl in Kharagpur city from 1991 to 2021. The urbanized area of Kharagpur town expanded significantly from 12.23% (5.40 sq. km) to 42.58% (18.70 sq. km) between 1991 and 2021. The LST study demonstrated that between 1991 and 2021, there was a notable fluctuation in the regional temperature trend. In October 1991, the highest temperature recorded was 28°C; by 2021, it had reached 36.51°C, reflecting an approximate increase of 8.5°C in Kharagpur city. The city was experiencing rising temperature trends due to significant urban expansion and industrial development. Key factors influencing urban expansion comprise the allocation of reclaimed land, comparatively low land costs, the benefits of open space at the city's outskirts, potential income opportunities, and a rapid escalation of industrial activity beyond the urban region. Consequently, the relevant authorities and inhabitants need to consider all useful and innovative strategies on an urgent basis to create a livable city for everyone.

Key Words: Urban sprawl, Shannon's entropy model, CA Markov chain model, LST



### Synthesis, characterization, and biological evaluation of heparin-capped carbon dots

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Abstract: In recent days, carbon dots (C-dots) have attracted tremendous interest amongst all carbon-based nanomaterials due to its unique electronic, optical and physicochemical behaviors. Carbon dots with very small size and uniform shape were synthesized by dehydration of Dglucose. The synthesized C-dots were subsequently stabilized by suspending in 0.5% (w/v) heparin solution. Surface plasmon resonance (SPR) band of Heparin capped C-dots (Hep-C-dots) was observed at wavelengths of 221 nm and 280 nm. Hep-C-dots have been characterized by TEM, XRD, FT-IR and zeta potential analyses. Hep-C-dots have small size  $(2.5 \pm 0.5 \text{ nm})$  with a narrow size distribution and high negative surface charge (-37.8 mV). The binding ability of Hep-C-dots with two important proteins of human body namely, human methemoglobin (HB) and human serum albumin (HSA) were studied in vitro with the help of fluorescence spectroscopy. To rationalize the nomination of heparin as capping agent, toxicity of Hep-C-dots towards normal peripheral blood mononuclear cells (PBMCs) were studied and compared with that of the bared C-dots. The outcomes revealed that Hep-C-dots did not exhibit significant toxicity justifying the efficacy of heparin as capping agent. Thereafter, we extended the toxicity study towards two tested cancer cell lines, Jurkat and K-562. The findings showed Hep-C-dots were less selective towards Jurkat and K-562 cells and their viability were reduced by 42% and 45% respectively when treated with 200 μg/ml Hep-C-dots. Thus, an acute toxicity of Hep-Cdots towards two tested cancer cell lines (Jurkat and K-562) and mild toxicity against PBMCs established it as a promising anticancer agent.



# Multiple emissions of benzil at RT and 77K and their assignments from *abinitio* quantum chemical calculations

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**Abstract**: Benzil exhibits multiple emissions under various conditions, including at room temperature in solutions and at 77K in low-temperature glass matrices. The emission properties at low temperatures were examined in rigid matrices frozen under various illumination conditions. This study presents a comprehensive analysis, integrating steady-state, time-resolved, and *ab-initio* quantum chemical calculations, to assign the various fluorescence bands of the fluorophore

molecule to distinct geometries and/or electronic states. The emission properties of benzil's skew form depend on excitation wavelength, with emission from both S1 and S2 states, whereas the relaxed trans-planar conformer emits only from the S1 state. A new emission band, peak in around 360 nm, has been attributed to the S2 state, shedding light on previously uncharted territory. Theoretical *ab-initio* calculations using DFT at B3LYP/6-31G\*\* level corroborate well with experimental results, validating this methodology.



# Synthesis of some new arylazo-coumarin derivatives and their comparative biological activity studies: Cytotoxicity, gene, DNA binding, BSA binding

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**Abstract:** In this study, four arylazo-coumarin derivatives (1–4) were synthesized via diazo coupling reactions, with compounds (2) and (3) being newly developed and structurally confirmed using various spectroscopic techniques. A comparative biological assessment was conducted to understand how the presence and position of a chloro substituent on the aromatic ring affect the biological properties of these azo-coumarin compounds. Both experimental and theoretical analyses indicated that compound (4) exhibits the highest biological activity, followed by compounds (2), (3), and (1).

Cytotoxicity assays on human glioblastoma LN-229 cells supported this trend, with compound (4) showing the most potent activity, while compound (1) appeared to enhance the viability of murine N9 microglial cells. DNA interaction studies revealed that all derivatives bind within the minor groove of CT-DNA, with compound (4) demonstrating the strongest affinity.

Additionally, all compounds were found to interact with bovine serum albumin (BSA), again with compound (4) exhibiting the strongest binding. Thermodynamic analyses, supported by isothermal titration calorimetry (ITC), confirmed the spontaneity and feasibility of the binding interactions, as indicated by favorable  $\Delta H^{\circ}$ ,  $\Delta G^{\circ}$ , and  $T\Delta S^{\circ}$  values.



# Structural and magnetic studies on Fe<sub>2</sub>CrAl Heusler alloy nanoparticles for spintronic applications

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Abstract: Half metallic ferromagnets (HMF's) are a prominent class of materials having their characteristic electronic band structure and magnetic properties, can be used potentially in the field of spintronics. Over the previous few years, Heusler alloys have been considered the most capable candidates for spintronics and magneto-electronics due to theoretical calculation of their half metallicity and high Curie temperature. Heusler compounds are ternary intermetallic compounds consisting usually of two transition metals (X, Y) and one main group element (Z). They can be divided into two groups having compounds with the chemical formula X<sub>2</sub>YZ and XY<sub>2</sub>Z having four fcc sublattices called Full Heusler alloy and Inverse Heusler alloy. However, Heusler nanoparticles (NPs) display wholly the majority of features to different extent. Hereafter it is value studying the fundamental features such as in what way the size and profile of NPs distress the physical properties of Heusler NPs. The present work investigates the effect of mechanical alloying on forming Fe<sub>2</sub>CrAl Heusler alloy and its structural and magnetic properties. The polycrystalline NPs of size 30 nm was synthesized from high purity precursors in the stoichiometric ratio using wet ball-milling method for 60 hrs followed by heat treatment at 800 °C for 24 hrs under argon atmosphere with heating rate 10°C/min. X-ray and selected area electron diffraction patterns have confirmed the cubic Heusler phase of the NPs with the A2disorder. These NPs are found to have low coercivity ( $H_C \sim 30$  Oe) indicating the soft magnetic property of the material, and exhibit a high saturation magnetization (Ms~ 53.7 emu/g) at low temperature. The high Ms and Curie temperature (Tc~ 315 K) make the present system a potential candidate for magnetically activated nano-devices working around room temperature.

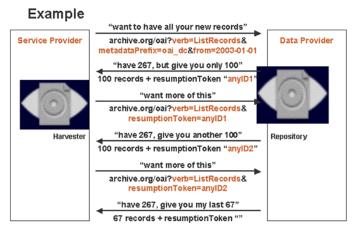


### Metadata Collection Technique in Digital Sphere

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Abstract: In digital sphere diversified data can found. In academic perspective metadata is became more important now a days to study the data about data. Metadata is structured, organized information about an object such as its source, scope, physical or digital. It used to Cross-walk through information about different subject materials. OAI-PMH is one of protocol used to collect this metadata. In DCMI DC data is retrieved through this protocol to further study in different literature. Six different verbs used for data collection via REST-API method. By this method mainly XML data retrieved. The XML data results can be varied depends over databases to databases. This technique is mainly used in academic study for doing different research of improvement of objects, repository framework, and crosswalks over different literature and quantitative study for further improvements. In the area information retrieval Descriptive



Metadata mainly used for academic study where other formats like structural metadata is used to describe the objects to maintain the framework and Administrative metadata is used to study and maintain for decision making and usability study for further improvements of services. This data collection technique is used to serve diversified fields of literature for research and development.

**Keywords:** Metadata, Data Collection, DCMI, Repository, OAI-PMH Protocol, REST-API, XML

#### **References:**

- 1. Brodie, E. (1988). Understanding M.E. *Nursing Times*, 84(31).
- 2. Jenn Rilley. (2014). *Understanding M Etadata What Is Metadata*, . http://www.niso.org/apps/group\_public/download.php/17446/Understanding Metadata.pdf
- 3. *Main Technical Ideas of OAI-PMH*. (n.d.). Retrieved April 23, 2025, from http://www.ukoln.ac.uk/metadata/oa-forum/tutorial/page3.htm#section3



# Fuzzy Interpolated Images Based Reversible Data Hiding Method using Modulo operation and Prediction-Error Expansion.

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**ABSTRACT:** In this study, a unique image interpolation method is constructed using the fuzzy weight strategy. The interpolated pixel values are generated by considering the fuzzy weight value of each pair of pixels in a selected block. The range between the block's minimum and greatest value has been represented by the fuzzy membership values of each pair of input pixels. The fuzzy output function receives the input membership value and uses the Max-Min composite principle to determine the strength of the fuzzy rule. The fuzzy output function is then used to compute interpolated pixel values based on the fuzzy rule's strength through a defuzzification process. Actually, fuzzy weight-based interpolation algorithms produce virtual pixels that are better than the currently employed interpolation methods. We suggest an RDH approach for interpolated images based on modulo operation and prediction-error expansion (PEE)in order to address significant image distortion in current approaches brought on by embedding based on interpolated pixels. Our approach is distinct from current RDH techniques that take into account data embedding into interpolated pixels. Initially, an interpolated image is created using an fuzzy image interpolation technique and divided into overlapping 3 × 3 blocks. Each block has secret data embedded in reference pixels using the PEE and interpolated pixels using the modulo operation. Here, 512 × 512 standard grayscale images were chosen as experiment input images from the well-known USC-SIPI, 2017 image collections. The studies' findings demonstrate that the recommended approach nearly always yielded the highest PSNR images. Therefore, the enhanced cover image was created utilizing the proposed technique by using the FWS with modulo operation and the reference pixel with PEE.



## Post-Human condition, man-machine association, and a 'scientific' forthcoming of humanities

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**Abstract**: Academia has lengthened its horizons in an exponential pattern in contemporary whiles, with inter-disciplinary associations becoming the pivotal force in nouveau research scopes. Hence, it has become necessary to de-classify disciplines from their sanctum of exclusiveness and create patterns, identify domains which intertwine various academic disciplines which seemingly are at collisions approach-wise. Contemporary studies in humanities have aligned itself with scientific disciplines in curving a new niche of research areas which not only enriches, but sustains the vitality of humanities as an academic area of interest. Posthumanities attempt to conjecture a situation where the present stage of the human condition is seen as a passing phase of human evolutionary condition which ultimately culminates into the evolved human of the future or the post-human. Moore and Moran defines post-humanism/the post-human as, "... an increase in technological development has drastically altered the possible means by which humans, nonhuman animals, and other objects can interact with one another. These advancements have ushered in new ways of producing knowledge in disciplines such as science and technology studies, animal studies, transgender studies, and new materialism." (Moore & Moran, 2016) Post-Humanist critiques envision a future beyond the anthropocentric vision, where nature, environment, and society co-habit to create a future which finally culminates in man-machine interface, defining the futuristic human form. Postmodern contemporary literature creates scenarios, fashions characters which are testimonios of a scientific human-future. As instances, one can cite modern superhero fictions with characters like the Cyborg (a human mind and heart, and part of human form encased within a mechanized exoskeleton), or a Swamp thing (an anthropomorphic plant-like eco-warrior crusading against global industrialization), which elevates literary genres from their cliched tones/treatment and provide a inimitable scientific outlook. The idea of co-existence of human and machines in modern science-fictions/films, their interdependency, futuristic writings like *Dune*, writers like Peter Cawdron or Becky Chambers have paved the way to link the discipline of humanities with its scientific counterparts, thus enriching its outlook, re-defining genres, and fostering research creativity. In a nutshell, several contemporary literary works/texts interweave the idea of literature with a proper scientific outlook/approach. This paper/poster shall look to deconstruct the traditional methodology of questioning humanities as a discipline, and probe into the contemporary research domains that intertwines it with subjects like genetics, physics, anthropology, bio-science, and other such parallel domains, thus certifying a 'scientific' future for itself.

Keywords: Post-Human, interdisciplinary, scientific, futuristic, literature.



# Composition and antioxidant, antimicrobial properties of water lily (*Nymphaea Nouchali*)

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Abstract: Nymphaea nouchali flower extracts and its solvent fractionates were exposed to physicochemical and fundamental phytochemical screening utilizing standard tests. The present study includes physicochemical and phytochemical examinations of the N. nouchali flower. The plant's flower extracts were subjected to a variety of qualitative chemical analyses, which revealed the presence of various phytoconstituents such as flavanoids, terpenoids, saponins, phenolic compounds, carbohydrates, tannins, and glycosides. Column chromatography of the DCM and CHCl<sub>3</sub> extracts was finished by solvent eluting strategies, and separated fractions were exposed to TLC study, where two compounds have been isolated as flavonoids with R<sub>f</sub> values of 0.80 and 0.74, respectively. The existence of different bioactive segments confirms the use of N. nouchali for different diseases by conventional experts. In-vitro radical scavenging actions of the various flower extracts of N. nouchali were executed, and the methanol extract uncovered the most scavenging power owing to polyphenolic cell reinforcement action, while pet. ether showed the least activity. The IC<sub>50</sub> Value of the extracts pet. Ether, CHCl<sub>3</sub>, EtOAC, Me<sub>2</sub>CO, EtOH, MeOH and H<sub>2</sub>O were found to be 53.243 μg/ml, 62.647 μg/ml, 60.056 μg/ml, 57.728 μg/ml, 58.941 μg/ml, 69.611 μg/ml and 65.742 μg/ml respectively. The free radical scavenging properties of different extracts were in the order of: Methanol > Water > Chloroform > Ethyl acetate Ethanol>Acetone>Pet. Ether. The investigation exposed explicit individualities for the specific herbal medication which will be helpful in distinguishing proof and quality control of the herbal drug.

**Keywords:** *Nymphaea nouchali*, physicochemical analysis, extraction techniques, phytochemical screening, invitro-antioxidant activity.



## Proximate Analysis and Elemental Profile of Samanea saman Flower Kalyan Sur

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Abstract: The flower of Samanea saman underwent an extensive analysis to assess its nutritional profile and elemental composition. Initial phytochemical assessments indicated the presence of bioactive substances such as alkaloids, flavonoids, saponins, sterols, tannins, and phenols, showcasing the flower's medicinal potential. The proximate analysis showed that the flower is abundant in carbohydrates (50.43%) and fiber (17.35%), with a moderate level of protein (11.17%) and a low fat content (5.78%), thereby making it a significant plant source for dietary purposes. The elemental analysis revealed the existence of vital elements, including sodium (13.21 mg/100g), potassium (16.54 mg/100g), calcium (11.89 mg/100g), and magnesium (8.72 mg/100g). Iron was also present in meaningful amounts (20.47 mg/100g), as well as trace elements like chromium, manganese, cobalt, and copper. Toxic heavy metals such as lead, cadmium, mercury, and arsenic were found in minimal quantities, emphasizing the need for careful monitoring of their presence in prospective food and medicinal uses. These results underscore the potential of the Samanea saman flower as a provider of bioactive compounds, minerals, and nutritional elements, with possible implications for health, nutrition, and pharmacological studies.

**Keywords:** Samanea saman; Phytochemical analysis; Proximate composition; Elemental analysis.

#### **References:**

- 1. K. Sur, A. Kispotta, N. K. Kashyap, A. K. Das, J. Dutta, M. Hait, G. Roymahapatra, R. Jain, T. Akitsu, Physicochemical, Phytochemical and Pharmacognostic Examination of Samanea saman, ES Food & Agroforestry, 2023, 14, 1011, doi: 10.30919/esfaf1011.
- 2. G. S. Kumar, S. D. S. Kumaran, Phytochemical, cytotoxicity and docking studies of Samanea saman, International Journal of Pharmaceutical Sciences and Research, 2019, 10, 1235-1240, doi: 10.13040/IJPSR.0975-8232.10(3).1235-40.
- 3. M. Hait, N. K. Kashyap, J. Deepak, A. Patel, Seclusion of bioactive components from flower of Samanea saman, Plant Archives, 2020, 20, 4581-4584.
- 4. M. Hait, A. Giri, A. Thakur, Preliminary Phytochemical Studies on Flower of Albizia saman, Pharma Science Monitor, 2017, 8, 1-7.



# The distinguishing effect of the magnetic states of cobalton the performance of single-molecule magnet behaviors in a closely related Co<sup>III</sup>Dy<sup>III</sup> and Co<sup>II</sup>Dy<sup>III</sup> complexes

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**Abstract:** The synthesis and characterization of heterobimetallic 3d-4f complexes, labelled as 1 and 2, derived from a Schiff base ligand formed through the condensation of 2-aminobenzyl alcohol with methyl-substituted o-vanillin are reported. Detailed structural analysis reveals that complex 1 features a Co<sup>III</sup>-Dy<sup>III</sup> assembly, bridged by two alkoxide groups, with an octahedral geometry around the Co<sup>III</sup> center and a DyO<sub>9</sub> coordination sphere for the Dy<sup>III</sup> ion. In contrast, under nearly identical reaction conditions, an intramolecular nucleophilic attack resulted in a slight modification of the ligand from H<sub>2</sub>L to HL', leading to the isolation of complex 2, which features a Co<sup>II</sup>Dy<sup>III</sup> core bridged by a pivalate ion. To the best of our knowledge, this is the first reported instance of a dinuclear Co-Dy system with variable oxidation states of the cobalt center, utilizing a ligand system derived from substituted o-vanillin and 2-aminobenzyl alcohol. Both complexes 1 and 2 exhibit field-induced slow relaxation of magnetization, where the distinct magnetic states of the cobalt center play a crucial role in these behaviors. Theoretical analysis reveals that the principal magnetic axis aligns with the shortest Dy-O bond in complex 1, highlighting the charge polarization effect from the diamagnetic Co<sup>III</sup> ion in tuning the crystal field around the Dy<sup>III</sup> ion and influencing its magnetic anisotropy. In contrast, the ferromagnetic interaction between Co<sup>II</sup> and Dy<sup>III</sup> ions in complex 2 plays a key role in reducing quantum tunneling of magnetization (QTM). This study broadens the exploration of Schiff base-derived 3d-4f complexes and their magnetic properties, showcasing the potential for further development in this area. The discovery of Co-Dy complexes with cobalt in the +3 oxidation state represents a novel contribution to the existing literature on Schiff base ligands derived from

\o-vanillin and 2-aminobenzyl alcohol and 3d-4f SMM behaviours as well.

**Reference:** A Panja, Z Jagličić, R Herchel, NC Jana, P Brandão, K Pramanik "The distinguishing effect of the magnetic states of cobalt on the performance of single-molecule magnet behaviors in closely related Co III Dy III and Co II Dy III complexes" *New Journal of Chemistry*, **2024**, 48, 20410-20422.



# An expeditious entry to catalyst free Beginelli reaction: Access to biologically important benzofuro [3,2] pyrimidine derivative.

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Abstract: Benzofuro [3,2] pyrimidines have varieties of biological activities like Tyrosine kinase inhibitor, Hsp90 inhibitor, Adenosine receptor antagonist etc. Due to its prominent biological activities, a numerous number of synthetic methodologies have been developed. Till date, catalyst free methodology is unrevealed. Herewith we have developed a catalyst free methodology for the synthesis of benzofuro [3,2] pyrimidine in nontoxic solvent. A vast gallery of the benzofuro [3,2] pyrimidine derivatives are prepared by changing substitution in starting materials. Both electron donating as well as electron withdrawing substituents on starting material are competent for this reaction and produced the corresponding benzofuro [3,2] pyrimidine derivatives in good to excellent yields. The product can be isolated by normal filtration and can be purified by simple crystallization process.

$$\begin{array}{c} X \\ X \\ N = XH \\ N = XH$$



## Artificial intelligence and machine learning in healthcare sectors Dr.Indranil Chakraborty

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Abstract: As far as health and lives of human beings are concerned, new technologies that provide more proficient, supportive, and quicker analysis to arrange a proper treatment plan in time are tremendously valuable. Artificial Intelligence (AI) has been proved to be potentially effective means to unveil enormously promising expanse that has already started changing the current scenario of the healthcare industry, starting from improvising the diagnostic advancement to improved care giving, and managing hospital capabilities as well. In healthcare sectors, AI refers to use composite algorithms intended to achieve specific output in an automated manner. The newly constructed algorithms, after the data being fed by scientists, researchers and doctors into computers, can review, interpret and even suggest solutions to complex medical complications. Among the endless application of AI and its subdivision in healthcare sectors, the three main areas include medical imaging, natural language processing of medical documents, and genetic information. Many of these areas focus on diagnosis, detection, and prediction. Artificial intelligence has therefore found its widespread utility that includes but is not restricted to medical diagnostics, clinical trials, personalised medicines and drug discovery, pain management and improving patient outcome etc. There is no denying of the fact that, with the advent of modern technologies, human beings have always attempted to adopt those for the wellbeing of the human civilisation. Healthcare sectors are no exceptions. These techniques provide promising applications as well as significant challenges. Initial adoption issues, data privacy concern, compliance to regulations, logical biasness, and resistance to pursue the technology are the key challenges to be overcome.

**Keyword:** Artificial Intelligence, Healthcare Sector, Advancement, Challenges



### Scientific Development and Sufferings of the Adivasis

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Abstract: India is a developing country. Any developing country needs industry and industry needs electricity. One of the most popular source of thermal electricity is coal, the reserve of which is declining everyday. That is why, India has taken the policy to produce 25% of its required electricity from nuclear energy by 2050, in 2020 which was 3.2% of India's total electricity. Being said, its not a bad goal or intention. But, like other minerals like buxaite and copper, uranium is also found in the areas where, or in the surroundings, Adivasi villages are located. Sad to repeat but, states of India have always failed to relocate or compensate Advasi people accordingly, and in the process created development refugees and migrants. Those who refuse to leave their ancestral lands, suffer a lot politically and physically. Their plight is always ignored. One of the most significant example is, the people of Jaduguda. Jadugura, once a very active uranium mine, was suspended in 2014 due to environmental protests. Though the mills are active and produce a large quantity of uranium waste through tailings surrounding Jaduguda town, which pollutes the water sources and other resources through radiation, which ultimately affecting the people of Jaduguda. My paper tries to find and relate the sufferings of the Adivasis with the Scientific and Technological Development in India.

Key words: Adivasi, Migration, Displacement, Development, Suffering



### Analysis of Ionospheric VTEC before Strong Earthquakes

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**Abstract:** For more than ten years, predicting earthquakes has been one of the most challenging targets for scientists. Before massive, destructive earthquakes, a variety of precursory has been seen and reported. Those phenomena can be divided into three categories: thermal, acoustic, and electromagnetic channels. In this paper, we focus mainly on the vertical total electron content (VTEC), which belongs to the electromagnetic phenomena. Basically, total electron content is the total number of free electrons between the GPS satellite and the receiver. Data from different stations (SWARM, Formosat/COSMIC, TSX, JASON, and GIM) are utilized to detect vertical total electron content before the mainshock. The results are different from each other, and the foremost reason for these differences is the vertical coverage range of the data sources. Regarding the data they provide, they have some advantages and disadvantages compared to each other. For example, when GNSS station locations are taken into account, GIM-VTEC data from observation data exhibits better quality for land areas compared to oceanic regions, but JASON provides high-quality VTEC data only for ocean regions. Although the COSMIC-RO data on the plasmaspheric part seems to provide more accurate results. However, severe errors should be eliminated using suitable methods because of the observation noise of the data generated from multi-instruments. Considering all of these factors, it might be possible to use all data sources to present global VTEC maps in a suitable manner.



# Chiral Bronsted Acid Catalysed Enantioselective Syntheses of Phthalides: Application in the Synthesis of Herbaric Acid

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$$X + CO_2Me$$

CHO

CHO

 $CO_2Me$ 
 $CO_2Me$ 

Abstract: Optically active phthalides, also known as isobenzofuranones, are widely found in both natural and synthetic compounds of considerable synthetic relevance and are associated with diverse biological activities. Many of these synthetic products display important pharmacological effects. The diverse pharmaceutical properties of these compounds are highlighted by their demonstrated anticonvulsant, antibacterial, anti-HIV, and anticancer activities. For instance, 3-butylphthalide has anticonvulsant properties; isoochracinc acid and herbaric acid have antibacterial properties. Over the past few years, many efforts have been directed toward the asymmetric synthesis of phthalides or isobenzofuranones. Herein, we have reported a chiral Bronsted acid catalysed enantioselective syntheses of phthalides via aldol-lactonization reactions. A variety of enantioenriched phthalides containing  $\alpha$ -diazoesters were afforded in excellent yields and with excellent enantioselectivities. The catalytic system is amenable to gram-scale synthesis of phthalides. The synthetic potential of this methodology has also been demonstrated by exploiting the reactivity of diazo functionality in the product. Additionally, a concise synthesis of herbaric acid has been accomplished by using this protocol.

**Key Words:** Chiral Bronsted Acid Catalyst, Phthalides, Aldol-lactonisation. Herbaric acid.