7th International Conference on

Frontiers in Chemical Sciences

Department of Chemistry
Indian Institute of Technology Guwahati
2-4th December, 2024

Abstract Book

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7th International Conference on

Frontiers in Chemical Sciences

Department of Chemistry
Indian Institute of Technology Guwahati
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Director, IIT Guwahati

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Message

Professor Aditya N. Panda
Chairman, FICS 2024
Head, Department of Chemistry, IIT Guwahati

I am happy that our department is organizing its seventh biennial international conference, Frontiers in Chemical Science (FICS 2024) from 2-4th December 2024. This conference provides an ideal platform to discuss the state of the art in chemical sciences and newer directions of research. In addition to having many younger and prolific researchers from India, like in previous editions, many international speakers are participating and delivering talks in FICS 2024, making the conference truly international. The FICS 2024 conference will deliberate on all branches of chemical science and engineering encompassing fields from theory and experiment to applications of chemistry to modern science and technology. Although the conference is devoted exclusively to the science and practice of chemistry but it will give participants a platform to exchange their ideas, discover novel opportunities, acquaintance with colleagues and to grow the network.

On behalf of the Chemistry Department, I am delighted to welcome all the delegates from India and abroad to IIT Guwahati. Success of any conference depends ultimately on many people who have worked in planning and organizing both technical program and supporting societal arrangements. In general, I thank the program advisors for their wise advice and brilliant suggestions on organizing the technical program the organizing committee for selecting active researchers. We take this opportunity to thank all our sponsors of the conference for their generous funding. I thank all the members of the local organizing committee of FICS 2024 for their hard work and wish a superb conference experience as well as an enjoyable stay in IIT Guwahati to all participants.

Program Schedule for FICS 2024

Day-1: 02-12-2024 (Monday)			
Time	**Events**		
7:30 – 9:00 AM	Breakfast & Registration *Venue: Conference Centre Foyer*		
9:00 – 9:30 AM	Inauguration and Photo Session *Venue: Conference Hall 2 and Administrative Building Foyer*		
9:30 – 10:00 AM	Tea break; *Venue: Conference Centre Foyer*		
10:00 – 10:40 AM 10:40 – 11:10 AM	PL-1: Prof. Mukundan Thelakkat KL-1: Prof. Joshua Philip Barham *Chair: Prof. Bhisma K. Patel* *Venue: Conference Hall 2*		
Conference Hall 2		**Conference Hall 3**	
11:15 – 11:35 AM 11:35 – 11:55 AM 11:55 – 12:15 PM	IL-1: Prof. Debayan Sarkar IL-2: Prof. Suman De Sarkar IL-3: Prof. Santanu Panda *Chair: Prof. A. T. Khan*	11:15 – 11:35 AM 11:35 – 11:55 AM 11:55 – 12:15 PM	IL-4: Prof. Rambabu Chegondi IL-5: Prof. Kuntal Manna IL-6: Prof. Sayantan Paria *Chair: Prof. Dipankar Srimani*
12:30 – 2:00 PM	Lunch Break; *Venue: Conference Centre Foyer*		
Conference Hall 2		**Conference Hall 3**	
2:00 – 2:20 PM 2:20 – 2:40 PM 2:40 – 3:00 PM	IL-7: Prof. Bani Kanta Sarma IL-8: Prof. Debashree Ghosh IL-9: Prof. Arun K. Manna *Chair: Prof. Ashish K. Gupta*	2:00 – 2:20 PM 2:20 – 2:40 PM 2:40 – 3:00 PM	IL-10: Prof. Rajiv K. Kar IL-11: Prof. Garima Agrawal IL-12: Prof. D. Mukherjee *Chair: Prof. Uttam Manna*
3:00 – 3:30 PM	Tea Break *Venue: Conference Centre Foyer*		
Conference Hall 2		**Conference Hall 3**	
3:30 – 4:30 PM	OP1-OP5: Student Oral Presentation *Chair: Prof. Krishna P. Bhabak*	3:30 – 4:30 PM	OP6-OP10: Student Oral Presentation *Chair: Prof. Debdas Dhabal*
4:30 – 4:50 PM 4:50 – 5:10 PM 5:10 – 5:30 PM	IL-13: Prof. S. Yaragorla IL-14: Prof. Animesh Das IL-15: Prof. Jagannath Mondal *Chair: Prof. Aditya N. Panda*	4:30 – 4:50 PM 4:50 – 5:10 PM 5:10 – 5:30 PM	IL-16: Prof. Indranil Chatterjee IL-17: Prof. Pankaj Chauhan IL-18: Prof. Nanda Dulal Paul *Chair: Prof. Chandan K. Jana*
5:30 – 7:30 PM	Poster Session (P1 – P155) *Venue: Conference Centre Foyer*		
7:30 – 9:30 PM	Dinner *Venue: Conference Centre Foyer*		
Day-2: 03-12-2024 (Tuesday)			
7:30 – 9:00 AM	Breakfast; *Venue: Conference Centre Foyer*		
9:00 – 9:40 AM 9:40 – 10:10 AM	PL-2: Prof. Dirk Volkmer KL-2: Prof. Michael Hirtz *Chair: Prof. Mohd. Qureshi* *Venue: Conference Hall 2*		

Conference Hall 2		**Conference Hall 3**	
10:15 – 10:35 AM	IL-19: Prof. S. Bhattacharyya	10:15 – 10:35 AM	IL-22: Prof. Ashutosh K. Mishra
10:35 – 10:55 AM	IL-20: Prof. Amit K. Paul	10:35 – 10:55 AM	IL-23: Prof. Debabrata Patra
10:55 – 11:15 AM	IL-21: Prof. Sayan Bagchi	10:55 – 11:15 AM	IL-24: Prof. Biswajit Saha
	Chair: Prof. Kalyanasis Sahu		*Chair: Prof. Gopal Das*
11:15 – 11:45 AM	Tea Break *Venue: Conference Centre Foyer*		
Conference Hall 2		**Conference Hall 3**	
11:45 – 12:05 PM	IL-25: Prof. Kingsuk Mahata	11:45 – 12:05 PM	IL-28: Prof. Subhabrata Maiti
12:05 – 12:25 PM	IL-26: Prof. Himansu S. Biswal	12:05 – 12:25 PM	IL-29: Prof. Benudhar Punji
12:25 – 12:45 PM	IL-27: Prof. Kalyan Raidongia	12:25 – 12:45 PM	IL-30: Prof. Samit Guha
	Chair: Prof. Jagannath Mandal		*Chair: Prof. Chandan Mukherjee*
12:45 – 2:30 PM	Lunch Break *Venue: Conference Centre Foyer*		
Conference Hall 2		**Conference Hall 3**	
2:30 – 2:50 PM	IL-31: Prof. D. Sureshkumar	2:30 – 2:50 PM	IL-33: Prof. E. Balaraman
2:50 – 3:10 PM	IL-32: Prof. Goutam Ghosh	2:50 – 3:10 PM	IL-34: Prof. P. Rajamalli
	Chair: Prof. Subhas C. Pan		*Chair: Prof. A. S. Achalkumar*
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Conference Hall 2		**Conference Hall 3**	
3:40 – 4:20 PM	OP11-OP14: Student Oral Presentation *Chair: Prof. Akshai Kumar A. S.*	3:40 – 4:20 PM	OP15-OP18: Student Oral Presentation *Chair: Prof. Pavan K. Kancharla*
4:20 – 4:50 PM	KL-3: Prof. Tapas K. Maji *Chair: Prof. Aditya N. Panda* *Venue: Conference Hall 2*		
4:50 – 6:50 PM	Poster Session (P156 – P309) *Venue: Conference Centre Foyer*		
7:30 – 9:00 PM	Conference Dinner *Venue: Conference Centre Foyer*		
Day-3: 04-12-2024 (Wednesday)			
7:30 – 9:00 AM	Breakfast *Venue: Conference Centre Foyer*		
9:00 – 9:40 AM	PL-3: Prof. Werner Nau		
9:40 – 10:10 AM	KL-4: Prof. Suvarn Kulkarni		
	Chair: Prof. Debapratim Das; Venue: Conference Hall 2		
10:20 – 10:40 AM	IL-35: Prof. Hari P. Nayek		
10:40 – 10:55 AM	Ind-1: Dr. Subhendu Pandit		
	Chair: Prof. Sujata Mandal; Venue: Conference Hall 2		
11:10 – 11:25 AM	Tea Break *Venue: Conference Centre Foyer*		
11:25 – 12:30 PM	Valedictory Programme		
12:30 – 2:00 PM	Lunch Break *Venue: Conference Centre Foyer*		
7:00 – 9:00 PM	Dinner *Venue: Conference Centre Foyer*		

PL: Plenary Lecture; **KL:** Keynote Lecture; **IL:** Invited Lecture; **OP:** Oral Presentation; **P:** Poster, **Ind:** Industrial Lecture

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Plenary Lectures		
SL No.	Speaker	Title of Presentation
PL-1	Mukundan Thelakkat	How to design polymers to fulfil functions in biosensors, thermoelectrics and batteries?
PL-2	Dirk Volkmer	Functional K3,3 (“Kuratowski”) Building Units in Materials Chemistry: Past, Present, and Future.
PL-3	Werner M. Nau	The Chaotropic Effect as an Assembly Motif in Chemistry
Keynote Lectures		
KL-1	Joshua Philip Barham	New Concepts in Visible Light-Powered Catalysis: Organophotocatalytic Dyads and Autophotocatalysis
KL-2	Michael Hirtz	Scanning Probe Lithography for Precision Chemical Surface Engineering and Device Functionalization
KL-3	Tapas K Maji	Solar Fuel Production through Post-Synthetic Modification of Metal-Organic Frameworks
KL-4	Suvarn S. Kulkarni	Are there sugars in bacteria? What can we do with them?
Invited Lectures		
IL-1	Debayan Sarkar	Can Visible Light Do Selective Dearomative C-H Activation
IL-2	Suman De Sarkar	Regulating Chemo- and Regio-selectivity through Controlled Electrolysis
IL-3	Santanu Panda	Exploiting α-Gem-Boryl Carbanions and Vinyl Boronates for Diverse Synthetic Applications
IL-4	Rambabu Chegondi	Cu(I)-Catalyzed Enantioselective Hydrocupration
IL-5	Kuntal Manna	Selective Methane Oxidation to Methanol or Acetic Acid using O_2 over Metal-Organic Framework Supported Abundant Metal Catalysts
IL-6	Sayantan Paria	Comparing the Electronic Structure and Proton-Coupled Electron Transfer Reactivities of CuIII and NiIII complexes of Bis-Amidate-Bis-Alkoxide Ligands
IL-7	Bani Kanta Sarma	Leveraging Local Interactions to Affect Global Structures of Peptides and Peptidomimetics
IL-8	Debashree Ghosh	Computational chemistry to understand light matter interaction
IL-9	Arun K. Manna	Modelling Intersystem Crossing in Metal-Free Organic Molecules for Efficient Triplet Photosensitization
IL-10	Rajiv K. Kar	Enhanced Surface Processes of Carbonaceous Materials with Biocompatible Riboflavin
IL-11	Garima Agrawal	Smart Biodegradable Microgels: A Versatile Platform for Diverse Applications
IL-12	D. Mukherjee	Frustrated Lewis Pair-Like Activation of Small Molecules by An Azomethine Ylide with a Counter-Intuitive Bias for CS_2 over CO_2.
IL-13	S. Yaragorla	Cyclizative Functionalization of Alkynols through Propargyl-Claisen Rearrangement
IL-14	Animesh Das	Design and Utilization of Metal Catalysts for Selective C-C and C-O Bond Forming Reactions
IL-15	Jagannath Mandal	Simulating Multi-substrate bound state of Cytochrome P450
IL-16	Indranil Chatterjee	Light-Camera-Action: Shining Visible Light on Hantzsch Ester
IL-17	Pankaj Chauhan	Harvesting Light for Developing Enantio-/Diastereo-/Chemoselective Transformations
IL-18	Nanda Dulal Paul	Ligand-Centered Redox Induced Chemical Transformations
IL-19	S. Bhattacharyya	Developing sustainable luminescent nanomaterials for solar to chemical energy conversions through complete metal free approach
IL-20	Amit K. Paul	Enhancement of Complexation due to the Bath Effect: A van der Waal Complex in N_2 Bath
IL-21	Sayan Bagchi	Probing surface-ligand interactions in SCN--capped quantum dots using 2D IR spectroscopy

IL-22	Ashutosh K. Mishra	Harnessing the photophysical nature of Flavin for biological applications
IL-23	Debabrata Patra	Autonomous fluidics: A chemically powered self-sustained motion.
IL-24	Biswajit Saha	Ferrocene functionalized bimetallic catalysts for water oxidation
IL-25	Kingsuk Mahata	From Discovery to Fluorescence Thermometer via H- to J-Aggregate Switching: the Journey of Aldrone Condensation
IL-26	Himansu S. Biswal	Probing Aromaticity with Hydrogen Bonding in a Supersonic Molecular Jet
IL-27	Kalyan Raidongia	Nanofluidic Flow through Bio-Channels; a Novel Resource of Sustainable Energy
IL-28	Subhabrata Maiti	Chemoselective Bioconjugation and Enantioselective Catalysis inside Protein Condensate
IL-29	Benudhar Punji	Catalytic Functionalization of Indole Derivatives Enabled by Iron Complexes
IL-30	Samit Guha	Development of Mechanically Interlocked Molecules for Targeted Imaging
IL-31	D. Sureshkumar	How Distal is Distal C(sp3–H) Activation?
IL-32	Goutam Ghosh	Tuning Piezoelectric Responses in Naphthalene Diimide Appended Peptides and Amino Acids through Controlled Self-Assembly
IL-33	E. Balaraman	Dehydrogenative coupling of alcohols with internal alkynes: An access to β-deuterated branched ketones
IL-34	P. Rajamalli	Regulating Spatial Configuration in Donor-π-Acceptor for Through-Space Exciton Transfer: Concentration-Independent Emitter for OLEDs
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OP2	Aniruddha Das	Design and Characterization of Nickel Complexes as Analogues for Nip Sites in Acetyl Coenzyme A Synthase/CO Dehydrogenase: Electrochemical and CO Reactivity Properties
OP3	Ankita Sarkar	DECON-impregnated hydrogel-based soft contact lens- a novel approach in inhibiting ocular herpetic inflammation
OP4	Anmol	Unveiling the Role of Solvent in Solution Phase Chemical Reactions using Deep Potential-Based Enhanced Sampling Simulations
OP5	Arup Samanta	Metal-Ligand Cooperation and Redox Promoted Alcohol Activation Using Zinc Complex
OP6	Geetanjali Deka	Fe(III)-Complex Incorporated and Surface-Modified Porous Silica Nanosphere as Hepatocyte-Targeted MRI Contrast Agent
OP7	Kshitiz Verma	$Sc(OTf)_3$-Catalyzed Domino C–C/C–N Bond Formation of Aziridines with Quinones via Radical Pathway
OP8	Mehak	Magnetic Nanoparticles as Magnetic Hyperthermia Agents
OP9	Nasireddy Seshadri Reddy	Photocatalytic, Intermolecular Olefin Alkylcarbofunctionalization Triggered by Haloalkyl Radical Generated via Halogen Atom Transfer
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OP11	Renitta Benny	Conformational control of Thiourea and Squaramides for ON/OFF Catalysis Regulation
OP12	Rikitha S Fernandes	Exploring the Synergistic Effect of Aggregation and Hydrogen Bonding: Fluorescent Probe for Dual sensing of Phytic Acid and Uric Acid
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OP14	Rubi Moral	Tripodal AIE active acylhydrazone based probe for selective turn on response towards Zn^{2+} in HEPES buffer and as anion/metal responsive organogelator
OP15	Sanskruti Smaranika Dani	Flexible PVDF-BST Electrospun Nanocomposites for Enhanced Piezoelectric Energy Harvesting

OP16	Soumitra Sau	Triphenylamine based CMPs as efficacious photocatalysts towards phenol production, simultaneous detection and degradation of micropollutants
OP17	Swarnalata Maity	MXene derived metal organic framework@PANI heterostructure as a hybrid supercapacitor
OP18	Uttama Mukherjee	A CO_2 Capture Journey through Computational Modeling – Amines and beyond
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IndL-1	Subhendu Pandit	An Introduction to Magritek's Spinsolve Benchtop NMR: Its Applications, From Academia to Industries
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P-2	Achinta Medhi	Microstructural analysis of reverse ATRP-prepared poly (butyl acrylate) grafted silicone rubber using various modes of NMR
P-3	Aditi Boruah	L-Proline catalyzed multi-component synthesis of N-pyridyl-tetrahydroisoquinolines and their α-C(sp3)-H oxygenation
P-4	Adyasa Sahoo	Is the Machine-learned mW (ML-mW) model better than the mW Model in representing water's Vapor-liquid Equilibrium?
P-5	Aftab Hossain Khan	Targeted Estradiol-Derived Carbon Dots for Selective Induction of Apoptosis in ER (+) Breast Cancer Cells via Oridonin-Activated p53 Pathway
P-6	Agrim Jhilta	Gelatin-Statin Microspheres to Modulate Immune Response and Counter Mtb-Induced Immunopathology: A Novel Therapeutic Approach to Target Tuberculosis Pathogenesis
P-7	Ahmad Ali	(Reactivity study of 4-hydroxydithiocoumarin with isocyanide "synthesis of (E)-3-((amino)methylene)-2-thioxothiochroman-4-one derivatives" and its cycloadducts)
P-8	Akshaykumar B. Wadhave	Cyclopropenium Salt Catalysed Dimerization of Styrenes
P-9	Akshi Deshwal	Chemotactic Directionality of Alkaline Phosphatase in the gradient of carbohydrates and metal ions
P-10	Alpana Sahu	Interplay of Capacitive and Diffusion Contributions in Redox Active Complex Metal Oxide Rods Channelled into MXene For Improved Charge Transfer Dynamics
P-11	Aman Singh	Photocatalyst-Free N-Arylation of Secondary Amines Under Visible-light Irradiation
P-12	Amon Das	Organotin (IV) derivatives with 2-hydroxy-5-((4-(trifluoromethyl)phenyl)diazenyl)benzoic acid: Synthesis and structures
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P-14	Anamika Bandyopadhyay	Photophysical and computational studies on an HSA selective D-π-A probe
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P-22	Ankita Sahu	Vanadium doped cobalt selenide: a potent oxygen evolution electrocatalyst
P-23	Ansalin Gnana Sowndarya A	Enhancing the flame retardancy of natural leather using carbonate-based inorganic salt: synthesis, characterisation, and application studies
P-24	Anurag Saini	Process development for the total synthesis of the novel drug metabolite Carboxy toremifene as a standard reference material along with characterization and purity assessment for the Antidoping quality Control Purposes
P-25	Anusaya S. Chavan	An efficient biocatalysed synthesis of 2-aryl chromones through oxidative cyclization
P-26	Anushka Rastogi	Ruthenium (II)-catalyzed C-H activation/annulation of pyrroline carboxylates with alkynes: synthesis of 2,3-diphenylspiro-[indene-1,2′pyrrolidine] carboxylate derivatives
P-27	Arati Chetry	Highly selective solution and film based sensor for colorimetric sensing of arginine in aqueous and blood samples.
P-28	Archana Chutia	Synthesis of Highly π-Extended Dihydrobenzo[a]indenocarbazole Scaffolds via Tandem Benzannulation and Friedel–Crafts Reaction of 2-Alkynylanilines and 2-Alkynylbenzaldehydes Promoted by Lewis Acid
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P-78	Giribala Madhavrao Bondle	Design, synthesis and molecular docking study of novel Triazole-Quinazolinone hybrids as antimalarial agents
P-79	Gopika Premanand	A Proton-Conductive Co(II)-Polyoxometalate Acts as a Precatalyst for Efficient Electrocatalytic Water Oxidation
P-80	Gouranga Mahapatra	NdCoO3 nanoparticles grown on reduced graphene oxide sheets as an efficient electrocatalyst for hydrogen evolution reaction
P-81	Gourav Kumar	Selective Synthesis of 1,2-Dithiophene-Substituted Benzimidazoles Using Zinc Oxide Nanoparticles under Mild Reaction Conditions
P-82	Gunanka Hazarika	Selective Phosphate Removal from Wastewater with pH-Responsive Covalent Organic Networks Capable of Morphological Changes
P-83	Guruprasad N Sawant	Lipase catalysed synthesis and antioxidant evaluation of dihydroindoloquinolines
P-84	Harsha K	Tarnish Resistance Mechanism in Ag-4Cu-2.5Zn-1Ge novel Alloy: A Comprehensive Experimental and Computational
P-85	Hemanga Bhattacharyya	Palladium-Catalyzed Substrate-Switchable ortho-C-H Alkenylation and Alkylation of Benzoic Acids using MBH Alcohols
P-86	Hirak Jyoti Baishya	In silico Investigation of β-Lactams as Possible Inhibitors of Spike Protein RBD of SARS-CoV-2
P-87	Hirak Jyoti Phukan	Manganese-Complex Catalyzed Sequential Multi-component Reaction: Enroute to a Quinoline-Derived Azafluorenes
P-88	Hrishikesh Rajbongshi	Precise Identification of the LUMO in Silanes: A Key to Understanding Molecular Properties
P-89	Indraneel Debnath	Remote control of supramolecular organization of butylated PNI
P-90	Itu Mallick	Substituent-dependent, Switchable Synthesis of Non-aromatic and Aromatic Heterocyclic Sulfones Using Visible Light
P-91	Jagnyesh Kumar Satpathy	Sulfur Ligated Iron(III)-Alkylperoxide Complex: Spectroscopic Insights and Mechanistic Studies of Electrophilic Hydrogen Atom Abstraction with Aldehydes
P-92	Jasline Joseph	Metal-Metal Oxide Nanoparticle Embedded Ecofriendly Film with Natural Enhancers for Food Preservation
P-93	Jaysri Das[a]	Modulating Hydrogen Bubble Adhesion for Improved Water Splitting
P-94	Jeevanantham Arumugam	A well-designed bimetal coordination networks for efficacious electrochemical detection of caffeine in beverages
P-95	Jerina Soibam	Packing polymorphism and symmetry non-equivalence in Co(II) complexes of flexible dicarboxylic acid of 4,4'-biphenol
P-96	Jharna Mahato	Synthesis of imines from the coupling reaction of alcohols and amines catalyzed by phosphine-free cobalt(II) complexes
P-97	Jinti Moni Kumar	Living photo-oligomerization behavior of diazaanthracene-derived macrocycle
P-98	Jyoti Devi	Controlling Energy of LUMO from Remote Site and it’s Effect on Electrochemical Property and Oxygen Atom Transfer Reactivity and O-H bond activation by Cu(II)-Nitrite Complexes

P-99	Jyotish Barman	Cooperative Rh/Chiral Phosphoric Acid Catalysed Diastereo- and Enantioselective [3 + 3] Cycloannulation: Access to Oxa-Bridged Indoles
P-100	Rajesh K	Impact of Gadolinium Phosphate ($GdPO_4$) and Various Cations (Li^+, Ca^{2+}, La^{3+}) on the NIR Reflectance of Bismuth Vanadate Pigment
P-101	Kailash Mohar	Low-valent Post Transition Zinc Metal Catalyst Bearing C-C Bond Formation Reactions
P-102	Kangkana Bezborah	Microscopic, Spectroscopic and Thermophysical Properties of Cocus nucifera Mediated Graphene Nanomaterials
P-103	Kangkana Chutia	A Versatile Pd-Catalyzed Alkyne Annulation Process for π-Extended Benzofulvene Synthesis
P-104	Karthika K	Novel molecular hybrids of EGCG and quinoxaline: Potent multi-targeting antidiabetic agents that inhibit α-glucosidase, α-amylase, and oxidative stress
P-105	Kashpar John Britto	Synthesis of Isoxazole Derivatives from Tri-Substituted Donor-Acceptor Nitrocyclopropanes
P-106	Kathakoli Roy	Orange Emitting Naphthalene Diimide based Luminogen for Fluorometric detection of Thiol through Click Reaction
P-107	Khongbantabam Sanatombi Devi	A simple, efficient procedure catalysed for Knoevenagel condensation and Michael addition by organocatalyst.
P-108	Koushik Barman	Synthesis of anti-Alzheimer agent taking raltitrexed as a lead
P-109	Kripangkar Choudhury	Carbonaceous surfaces as drug delivery system: A DFT study
P-110	Kshitij Rawat	Development of Lignin-Derived Gold-Titanium Dioxide Nanocomposites for Light Assisted Antimicrobial Photodynamic Therapy
P-111	L.Ramapriya1	Band gap and Crystallite size Controlled ZnO Nanoparticles with Al, Zr and Se Dopants for Efficient Visible Light Photo Catalytic Remediation of Food Colorants Polluted Aqueous Systems at 250C
P-112	Madan Kumara	Tunable Reactivity of 2-Alkynylanilines toward N-Heterocyclic Compounds Synthesis
P-113	Madhab Barman	Palladium Catalysis Enabled Sequential C(sp3)−H/C−C Activation: Access to Vinyl -Lactams
P-114	Maitery Yadav	Salt-Tolerant, Protease-Stable and Non-Resistance Developing Cationic AMPs for Combatting Planktonic MRSA and its Biofilms
P-115	Malay Das	Synthesis of Sulfur Functionalized Isoindolone Scaffolds from Hydroxyisoindolinones
P-116	Malay Kumar	Reconstructing Functional Protein from its Fragments
P-117	Mangalassery P Athira	Tris(aryl)-cyclopropenium-ion Catalysed Bis-vinylation of Aldehydes
P-118	Manisha Sadangi	Ruthenium doped cobalt sulphide electrocatalyst derived from ruthenium-cobalt Prussian blue analogue (RuCo-PBA) for enhanced hydrogen evolution reaction (HER)
P-119	Manisha Sharma	Desymmetrization of 2,5-Cyclohexadienones via Organocatalyzed Asymmetric Domino Reaction: Direct Entry to the Hydrophenanthren-2(1H)-ones
P-120	Maniya V. Nanjegowda	Palladium-Catalyzed Weak Chelation-Assisted Site-Selective C-H Arylation of N-Aryl Pyridones via 2-fold C-H Activation
P-121	Manjunath R	Design, Synthesis, Computational studies, and evaluation of In-vitro anti-breast cancer potentials of Benzo[d] [1,3] dioxole and 2-Bromofuran tethered 1,2,4 triazole hybrids
P-122	Md Badirujjaman	Esterase-responsive Self-immolative Prodrugs for the Sustained Delivery of the Anticancer Drug 5-Fluorouracil with Turn-on Fluorescence
P-123	Meetkumar Y. Chaudhary	Water-Stable Metal−Organic Framework for Highly Sensitive and Selective Sensing of Metal Ions and Organo-toxin in aqueous Medium with Theoretical Revelation
P-124	Megha Parmar	Synthesis and Characterization of Sustainable Zeolite 4A from Kutch Kaolin Clay for Water Remediation: Enhanced by Machine Learning
P-125	Minaz Parbin	Construction of Structurally-Complex Multi-Component Coordination Cages

P-126	Mira Jhawar	Utilizing Human Calcitonin (hCT) to Prevent the Aggregation of Small Peptide Fragments 0f SARS-COV E-protein: A Computational Approach
P-127	Monika Gaur	Strategic Disruption and Inhibition of Amyloid Fibrils via Macrocyclic Templated Silver Nanoparticles
P-128	Monisha Venkatesan	A hierarchical porous sheets of bimetallic terephthalate frameworks for sensitive detection of theophylline drug
P-129	Mousumi Narzary	Synthesis of Zn3V2O8/g-C3N4 heterojunction for efficient photocatalytic degradation of water pollutants
P-130	Mridul Boro	Unconventional Supramolecular Assemblies in Metal Organic Multi-component Compounds of Ni(II), Co(II) and Mn(II): Combined Experimental and Theoretical Studies
P-131	Mrinal Kanti Kar	β-Carboline-based light and pH dual stimuli-responsive ion transporters induce cancer cell death
P-132	Mrityunjoy Dey	Bioinspired Nanoconfinement of Restacked Lamellar Nanofluidic Ni(OH)2 membrane for Enhanced Organic Transformation
P-133	Mukesh Jaiswal	Metastable [2]Rotaxane for Selective Fluoride Anion Detection
P-134	Mukesh Kumar	A Visible-light promoted synthesis of substituted benzo[c]-chromeno[4,3,2-gh]phenanthridine involving hetero-cross-coupling cyclization and aromatization reaction
P-135	Muralidhar	Deciphering the Antibacterial Action of Bis-Benzimidazole Derivatives through Docking and Molecular Dynamics Simulations on DNA-Topoisomerase-IA
P-136	Mwina Basumatary	Molecularly imprinted electrochemical sensor based on a metal organic framework-functionalized MWCNTs composite modified electrode for selective uric acid detection
P-137	Anjana Singha	Ultra-thin Dielectric Triggered Charge Injection Dynamics for High-Performance Metal Organic Framework/MXene Supercapacitors
P-138	Nabam Tayuma	Theoretical Investigation on Atmospheric Fate of CH3CH2C(O)OCH(O)CH3 Radical
P-139	Nabamallika Nath	Synergetic Combination of Bio-Electrolytes and Bio-Fluidic Channels as a Novel Resource of Sustainable Energy
P-140	Nakul Desai	Manganese empowered covalent organic polymer composite: Innovative Composite Materials for Next-Generation Energy Storage
P-141	Namrata Kumari	Nano-size zirconium oxide as an efficient adsorbent and a photocatalyst in visible light
P-142	Nandini Ray	One pot Metal-free synthesis of Aryl Fluorenones
P-143	Naorem Wangamba Singh	Extraction, isolation and characterization of pure compound from the leaf of the Phlogacanthus thyrsiformis
P-144	Naveen Kumar Kottakki	TYPE-C silica-hydride columns can perform ANP, RP and ONP and Adenine nucleotides separated in UDA (Undecanoic acid) Chemistry by HPLC-RP Method
P-145	Nayana Mukherjee	Piezoelectric Nanomaterials for Ultrasound-Mediated Therapy
P-146	Nazir Ud Din Mir	A Thiophene Functionalized Hf(IV) Organic Framework for the Detection of Anti-Neoplastic Drug Flutamide and Catalysis of Friedel-Crafts Alkylation
P-147	Nazir Uddin	Formation of Bis-indolylmethanes from Symmetrical Triarylmethanes via Brønsted Acid Catalyzed C–C Bond Breaking Reaction
P-148	Neeharika Baruaha	Unveiling Hetero Atom Containing Fluorescent Carbon Dots from Indigenous Soil Bacterial Metabolites for Toxic Cr (VI) Ion Detection
P-149	Neha Barnwal	White Light Emission from Zn(II) and DMSO-Induced Copper Nanocluster Assembly
P-150	Neichoihoi Lhouvum	Synthesis and characterization of liquid crystalline amide and ester bond containing benzo[1,2-g:3,4-g’:5,6-g’’]triquinoxaline core compounds
P-151	Nidhi Sharma	Layer-by-layer assembled Flexible Biosensor for On-Site Monitoring of Escherichia coli

P-152	Nijara Das	Mgo-Supported Sulfonated Graphitic Carbon Nitride: An Efficient Acid-Base Bifunctional Catalyst for One-Pot Deacetalization-Knoevenagel Cascade Reaction
P-153	Nikita Pala	Thiazolidinedione- and Triazole-based Synthetic Organoselenocyanates: Potential Anticancer Activities Against Triple-Negative Breast Cancer
P-154	Nikita Varghese	Fluorescent schiff base sensor for selective detection of co(ii) : applications in real sample analysis and cytotoxicity studies
P-155	Niku Moni Das	Evaluation of mode of indoleamine 2,3-dioxygenase 1 inhibition by 4,7-dichloroquinolines
Poster Presentations (Day-2)		
P-156	Nilja George	Aqueous Based Ultra-Small Magnetic Doped Semiconductor as a Potential Dual Imaging Probe in Biomedicine
P-157	Nisha Rawat	Photocatalyst Free Visible-Light-Induced Fluoroalkylative Oximation of Aryl Olefins
P-158	Nishant Mishra	Engineering the Molecular Structure of 6-gingerol for Ceasing the Human Lysozyme Idemic Condensates
P-159	Nishtha	The Hidden Chemistry of Weeds: Unveling Phytochemicals for Nutritional and Therapeutic Benefits
P-160	Nitish Saini	Photocatalytic CO2 Reduction to Methanol Integrated with the Oxidative Coupling of Thiols to S-X (X=S, C) bond formation over Fe3O4/BiVO4 Composite
P-161	Nitul Kalita	Hollow Cuboidal Metal Oxide-Based Asymmetric Electrode Configuration for High-Performance Anion Exchange through Quaternized Pyridine-Poly(vinyl alcohol) @ Metal Hydroxide Nanosheets for Water Dissociation
P-162	Sorokhaibam Nungshithoi Devi	Interaction of metal ions with two schiff bases of salicylaldehyde
P-163	Oiyao Appun Pegu	Micelle-assisted ultrafast sensing of cyanide via twisted-intramolecular-charge-transfer based fluorogenic nano-probes
P-164	Palak Mandal	Conformation-dependent excited state properties in extended π-conjugated systems
P-165	Pallav Jyoti Arandhara	A Lewis Acid-Catalyzed Cascade Synthesis of Fused N-Heterocycles from 2-Alkynylanilines and 2-Formylbenzonitriles: Unveiling Iminoisoindoloindolone and Its Derivatives
P-166	Pallav Mondal	Bimetallic MOF Templated Nanocomposites of Molybdenum Oxide for Water-Splitting
P-167	Pallavi Barman	Synthetic Benzylic Diselenides and Disulfides: Potential Anticancer Activities via Modulation of the ROS-Dependent Akt/β-Catenin Signaling Pathway
P-168	Paltan Laha	Two Sustainable Pathways of MOF-Catalysed Room Temperature Chemical Fixation of CO2 Inside Alkynes Under Atmospheric Pressure
P-169	P. Kumar	Detailed Studies on the Photoluminescence Properties of Wet Chemically Grown Eu-doped Wrinkled ZnO Nanorods
P-170	Parbin Rahman	Iodine Promoted N-acylation of sulfoximines via Oxidative C=C Bond Cleavage of Cinnamic Acids
P-171	Parijat Pratim Das	Fabrication of robust and versatile ionic thermoelectric devices of natural clay minerals
P-172	Partha Pratim Borah	Potential-dependent Oxygen Evolution Reactions on Fe-NC Materials
P-173	Partha Pratim Nath	First Asymmetric Total Syntheses of Avapyran and Dysiquinol D
P-174	Parvathy M U	Tuning Proton Conductivity in MOF-GO Composites by Modulating Graphene Oxide Content
P-175	Parveen Kumar	Selective N-Arylation of Thiopurine using C-F Bond Activation of Fluorobenzene: Emerging Drug against Prostate Cancer
P-176	Phuntso Gombu	Alcohol Dehydrogenases and their Potential Applications

P-177	Pinku Sarma	Dichalcogen, Halogen and Charge Assisted Hydrogen bonded Assemblies in Pyrazole-based Coordination Compounds of Ni(II), Mn(II) and Cu(II): Anticancer Activities and Theoretical Studies
P-178	Plabana Phukan	"Degradation of e-wastes using carbohydrates in water"
P-179	Ambuj Kumar Kushwaha	Visible-light-initiated Sulfonylation of Phenylhydrazines with Thiols
P-180	Poorvi Gupta	Metal−Organic Framework-Supported Mono Bipyridyl−Iron Hydroxyl Catalyst for Selective Benzene Hydroxylation into Phenol
P-181	Prabhat K. Maharana	Cobalt-Catalyzed Stereospecific C-N/C-O Bond Formation of Oxiranes with Diaziridines
P-182	Pragya Trivedi	Nuclear targeted triazole-bridged biotin-conjugated quinoline derived Single component organic nanoparticle-based two photon-responsive Drug Delivery Systems
P-183	Pranjal Das	Tuning of Electrocatalytic Water Oxidation Activity of Cu (II) Complexes by Changing Electron Donating Nature of Ligand Frameworks
P-184	Pranjit Saikia	Regio- and stereoselective synthesis ofAllylsulfones using DABCO
P-185	Prasanjit Agasti	Investigation of Magnetic and Magnetocaloric Properties in disordered Spinel Compound Fe2− xCuxSnS4
P-186	Prashant Kukreti	A multi-component synthetic route for 2-pyrazolines via acceptorless dehydrogenation of alcohols using homogeneous Ni(II) catalysts
P-187	Pratibha Mittal	Spectrophotometric Investigations of Charge Transfer Complexes formed between 1,2,4-triazoles and different acceptors: An Experimental and Theoretical Investigations
P-188	Prerna Chettri	Programmable Nano-Oscillators Engineering for Dual-State Emission in Solution and Solid Phases
P-189	Priti Bera	A Reusable MOF Coated Chitosan@Paper Strip Composite for Real-Time Monitoring of Pesticide Pendimethalin and Organo-Arsenic Feed Additive Roxarsone Levels in Environmental Water, Food and Vegetable Samples
P-190	Pritishree Panigrahi	Harnessing reductive BF2-complexation via Ru(II)-catalyzed N□O cleavage of isoxazoles
P-191	Priya Jayathsena R	Aza Phenalenone Derivatives Using Aldrone Condensation and their Applications
P-192	Priya Mahaur	Enhancing C–S and C–N bond formation with ultrasound assistance: lipase-catalyzed synthesis of 2,4-disubstituted thiazole derivatives from arylethanones and thioamides
P-193	Priya Yadav	Surface-Engineering of CaTiO3 for Photocatalytic Hydrogen Evolution Reaction through Enhanced Oxygen Vacancy
P-194	Priyam Das	Time-Encoded Information Encryption with pH Clock Guided Broad-Spectrum Emission by Dynamic Assemblies
P-195	Priyanka Pradhan	Frustrated Ion Pair Interactions Driven Anion Assisted Concerted Addition of Ketoximes/Aldoximes and Hydroxamic Acids to Glycals
P-196	Priyanka Ray	Improving the electrocatalytic activity of NiTe nanoflakes by coupling CeO2 for oxygen evolution reaction
P-197	Priyanka	Valorisation of rice straw into a valuable pigment: prodigiosin
P-198	Priyanku Nath	ROP of Quinazolinones to Polyacylamidines using a Cesium Catalyst
P-199	Puja Garai	Janus nanoparticles for enhanced cell uptake and drug delivery
P-200	Pulak Pradhan	CeO2-Mn3O4 Solid Solutions: Efficient Photocatalyst towards Degradation of Phenolic Compounds
P-201	Pulakesh Borah	Photoenhanced intrinsic peroxidase-like activity of metal free biocompatible borophene photonanozyme for colorimetric sensor assay of dopamine biomolecule
P-202	RK Bidyasana	Designing of Anthraquinone based flexible dicarboxylic acid[3-(carboxymethoxy)-9,10—dioxo-9,10-dihydro-anthracen-2yl]glycine and desingning co-crystal.

P-203	Mahendra K. V. Rotta	Direct Stereoselective Synthesis of 2-Deoxyglycosides via Visible-Light Induced Photoacid Catalyzed Activation of Glycosyl o-[1-(p-MeO-Phenyl)vinyl]benzoates (PMPVB) as Donors
P-204	Rahul Kesarwani	Stimuli-responsive biotin-anchored prodrug for targeted delivery of anti-cancer agent NBDHEX with turn-on NIR fluorescence
P-205	Rahul, P. Rajamalli	Self-assembled photosensitizer as photo-switchable oxidase mimic
P-206	Rajashree P. Mishra	Design of Ceria Nanoparticles Decorated MXene Photocatalysts to Drive Selective and Efficient Photoreduction of CO2 to Ethanol
P-207	Rajashri Sarmah	Designing Cobalt(II) Complexes for Tandem Dehydrogenative Synthesis of Quinoline and Quinazoline Derivatives
P-208	Rajesh Kushwaha	D-A-D-based Dinuclear Tridentate Ru(II) Complex with Strong Near-Infrared Light-Triggered Anticancer Activity
P-209	Rajneesh Kuldeep	Design And Synthesis of a POD-mimicking Bionanozyme as Colorimetric Probe for Neurotransmitter Detection
P-210	Raju Mandal	Base-Induced Decarboxylative 1,1-Alkoxy Thiolation via Hydrothiolation of Vinylene Carbonate
P-211	Rakshitha K Jain	Sustainable offset ink using Fluorene-Based Schiff base pigment for anti-counterfeiting and latent fingerprint detection
P-212	Ramkumar K	Beyond the Chain: Impact on Charge Transport in a π-stacked Polymer in Organic Electronics
P-213	Ranjana M	Fluorene-Conjugated Naphthalimide: A Novel Fluorescent Probe for H_2S Sensing and Cellular Imaging
P-214	Raseswari Dash	Efficient Synthesis and Structural Insights of a New Class of Benzo-extended Thia-quasi[7]Circulenes
P-215	Ravendra Kumar	Synthesis, Characterization, and In-silico studies of Hydrazide-hydrazone linked Coumarin Glycoconjugates
P-216	Reek Mahapatra	All-Liquid Transistor via Topochemically Polymerized chiral Interface Architectures for NO_2 Sensing
P-217	Ria Deb	Bimetal embedded nitrogen-doped carbon derived from conjugated macrocyclic polymers as electrocatalysts for oxygen reduction reaction
P-218	Richa Agrawal	Tetraarylpyrrolo[3,2-b]pyrrole-BODIPY dyad: A Molecular Rotor for FRET based Viscosity Sensing
P-219	Ritu Sharma	Unveiling the Bioactive Potential of Indian Adzuki Bean (Vigna angularis) for Nutritional and Health Benefits
P-220	Ritvika Kushwaha	Development of a Two-Step Sensitive Fire Alarm System Using Fire Retardant Cotton-Based Materials
P-221	Roshini N	Synthesis of Ca-Al Layered Double Hydroxide-alginate beads with potential application as adsorbent for water/wastewater treatment
P-222	Sabareeswaran Meyyanathan	Surface-Modified Tremella Flower Resembling Mixed Metal-oxide Microsphere as Effective Active Materials for Energy Storage
P-223	Sachin Sreedhar	Efficiency enhancement of porous coordination polymers based supercapacitor by implementation of organic redox mediator
P-224	Sadia Nudrat	Construing the interactions of coumarin derivatives with the main protease of stomach pepsin using spectroscopic and computational analyses: insights into the binding thermodynamics, anti-fibrillation studies and enzymatic assay
P-225	Sagar Srivastava	Solute Dynamics of a Hydrophobic Molecule in Menthol-Thymol Based Type-V Deep Eutectic Solvent: Effect of Composition of the Components
P-226	Saigal	An efficient and eco-friendly synthesis of novel nitro functionalized pyrroles and 1,4-dihydrpyridines using DMAP as an efficient catalyst
P-227	Samantha Da Costa	Nanostructural Characteristics and Oxidative Reactivity of Diffusion Flame Generated Soot using Methyl Crotonate and Methyl Butyrate as Surrogate Fuels
P-228	Samarpita Das	MnO2 Nanorods on Mesoporous Carbon as a Bifunctional Electrocatalyst for Hydrazine Oxidation and Oxygen Reduction Reactions in Alkaline Media

P-229	Sampurna Routray	Fabrication of a pH-responsive Moisture-sensitive Actuator for Humidity Detection
P-230	Sana Quraishi	Elucidation of inhibitory effects of bioactive anthraquinones towards formation of DNA advanced glycation end products (DNA-AGEs)
P-231	Sandeep Jat	QbD driven extraction, isolation and purification of piceatannol from passion fruit seeds and its cubosomes development, characterization and neuronal cellular analysis
P-232	Sangavi.V	Development of Phosphate Modified Inorganic Layered Double Hydroxide Based Eco-friendly Flame-retardant for Leather
P-233	Sanjana Banerjee	Fe(III)-incorporated porphyrin-based porous organic polymer as a peroxidase mimic for the sensitive detection of glucose and H2O2
P-234	Santu Mandal	Dual C(sp3)–H and C(sp2)–H Activation of 8-Methylquinoline N-Oxides: A Route to Access C7–H Bond
P-235	Sapana Sinha	Deciphering the Influence of Zwitterionic Surfactants on Pluronic Co-assemblies: A Synergistic Odyssey through Spectroscopic, Microscopic, and Scattering Techniques
P-236	Sarvesha S. Shetgaonkar	Design and Synthesis of Novel Heterogeneous Catalyst for the Carbonylation of Glycerol-to-Glycerol Carbonate with Urea
P-237	Sarwar Parvej	Room temperature columnar self-assembley of luminescent perylene based molecules with cyanovinylene chromophore
P-238	Sayon Satpati	Aromaticity of Polycyclic Conjugated Hydrocarbons in the Excited States – A Quantum Mechanical Approach
P-239	Sebastin Raj Jeny	Caesium Carbonate-Promoted Reaction of Nitro-Substituted Donor-Acceptor Cyclopropanes with Primary Aromatic Amines in Water: Access to β-Enamine Malonates
P-240	Seema Jangir	2D NiO/g-C3N4 nanocomposite for Photoelectrochemical Water-Splitting for Oxygen evolution Production
P-241	Sesadeva Mallick	ACO/Ag/MFO n-n Heterostructure for Photocatalytic Applications
P-242	Shabin N. Chathangad	Membrane-active amphiphilic EGCG derivatives and their silver nanoformulations as broad-spectrum antibacterial agents
P-243	Shagufta Gull	Core Diameter influence in NiO@Fe3O4 for Oxygen Evolution Reaction
P-244	Shaifali Bhardwaj	Magnetic β-glucosidase-inorganic hybrid nanoflowers: Highly active and recyclable nano-biocatalyst for cellobiose hydrolysis
P-245	Shalini Gupta	Electrochemical NH-Sulfoximidation with α-Keto Acids
P-246	Sharajit Saha	Ru-Catalyzed Redox-Neutral Coupling of N-Chlorobenzamides with Unsymmetrical Alkynes in Water
P-247	Shefali S. Ainkar	Biosynthesis of silver nanoparticles using Connarus monocarpus plant extract and its application as melamine sensor
P-248	Shibaditya Kumar	Analogues Copper Nanoclusters (Cu16/17) with Two Electron Superatomic and Mixed-valent CuII/CuI and CuI /Cu0 Characters
P-249	Shikha Pandey	Visible-light promoted Synthesis of Schiff Base via C-N bond formation: Benzyl Alcohol as an alternative of Aryl aldehydes
P-250	Shimna.M	MnO_2/PPy Hybrid Electrode; Advanced High-Performance Supercapacitors
P-251	Shreemoyee Phukan	Analysis of Physicochemical Parameters of Ground water around Silapathar and Simen Chapori Area of Dhemaji district, Assam
P-252	Shrodha Mondal	A carbon nanodot-based torch for detecting carbon monoxide
P-253	Shrutipriya Devi	Highly conductive multifunctional Iron incorporated Polythiophene nanocomposite: A nanocatalyst for nitrobenzene reduction in aqueous medium and an efficient room temperature methanol gas sensor
P-254	Shubhranshu Mishra	A ratiometric luminescent Tb(III) complex for efficient sensing of anthrax biomarker “DPA”
P-255	Siddhi K. Salgaonkar	Microwave Assisted Syntheses of Indolo[2,3-b]quinoline Scaffold containing heterocyclic compounds and the Alkaloid Neocryptolepine

P-256	Simant Kumar Srivastav	Multiferroic BiFeO3 nanoparticles as an efficient photocatalyst for sunlight-driven photocatalytic removal of textile dyes
P-257	Simran Sharma	Cost-effective Computations of Gold Standard of Quantum Chemistry
P-258	Sk Sakir Hossain	A Recyclable MOF@polymer Thin Film Composite for Nanomolar On-Site Fluorometric Detection of Heavy Metal Ion and Anti-Histamine Drug
P-259	Sk Taslim Ali	Impact of Dopant Concentration on the Growth Kinetics of Carbon Nanotubes
P-260	Smiti Rani Bora	End group modulation of A-D-A type small donor molecules for DTP based organic photovoltaic solar cells: A DFT approach
P-261	Sneha Paul	NiFe2O4@Chitosan-Anchored Magnetically Retrievable Cu(II) Schiff Base Complex: A versatile catalyst for Multicomponent Reaction
P-262	Sneigitha G	Enhanced Performance of πconjugated Metal Complex (TPZn) in Organic Field Effect Transistors
P-263	Sonakshi Bedi	Synthesis of Functionalized Tetralones and Naphthoquinones via Tamura Cycloaddition of Rauhut-Currier (RC) adducts of nitroalkenes with homophthalic anhydrides
P-264	Sonali Roy	Fabrication of Robust Forward Osmosis Membrane by Assembling Weakly Magnetic FeOxCly Nanoparticles
P-265	Sonam Kumari	Influence of Zn substitution into Ni-Co ferrite system and study its Structural, Magnetic and Supercapacitance properties
P-266	Soni Devi	Synthesis of CF3CH2-Amides/Propiolamides/Acrylamides: The TfOH Catalyzed Reactions of Nitrile Compounds with CF3CHN2
P-267	Soumya Srimayee	Synthetic Ion Transporter and its therapeutic application
P-268	Srija Ghosh	Nitrogen and Sulfur co-doped Carbon Quantum Dot decorated Ti3C2Tx-MXene as electrode material for high-performance symmetric supercapacitors
P-269	Srijan Mukherjee	A Post-Synthetically Modified Cationic, Robust MOF Featuring Selective Separation of Carboxylate Containing Pharmaceutical Drugs from Water at Neutral pH: Elucidation of Adsorption Mechanism by Theory and Experiments
P-270	Subhashree Sahu	Reversible CsPbBr3 ↔ CsPb2Br5 Transformation via Reverse Micellar Aqueous Solution
P-271	Subhasish Ray	LiBr-Promoted Reaction of □-Ketodithioesters and Thioamides with Sulfoxonium Ylides to Synthesize Functionalized Thiophenes
P-272	Subhasish Sahoo	Study of Structural Phase Transition and Optical Properties in a Series of New 0D Hybrid Metal Halides: (3,5-DMP)2Bi1-xSbxCl5
P-273	Subhradeep Kar	Copper-catalyzed (4+3)-cycloaddition of 4-indolylcarbinols with aziridines: stereoselective synthesis of azepinoindoles
P-274	Sudeshna Pal	Nanoscale Synergy: Harnessing Supramolecular Nanogel-Carbon Dots Conjugate for Enhanced Cancer Treatment through Combination Therapy
P-275	Sumanta Bera	Sulfur-tuned MoS2 quantum dot decorated Ti3C2Tx (MXene) electrode materials for high performance supercapacitor applications
P-276	Sumran Raikwar	The Z-enoate assisted Meyer-Schuster rearrangement (MSR) as a tool for the construction of vinyl sulfides
P-277	Sunanda Dogra	Application of Crystal Engineering in the Dimerization of C=N Bond
P-278	Suprakash Rabha	Sustainable Fabrication of WO3 Nanodices for Enhanced Ciprofloxacin Degradation
P-279	Supriya Manna	Non-template Synthesis of Furo[2,3-b]pyrrolo[2,3-d]pyridines via Pd(II)-Catalyzed Dual N−H/C Annulative-Cyclization
P-280	Suraj Kumar Agrawalla	Argentophilic Interaction in 6-chloro-7-methylpurine: Role of Anions in Structural, Electrical and Ionic Properties
P-281	Suruchi kumari	Synthesis of SMAC mimetics for the treatment of cancer
P-282	Susanta Mandal	Pharmacophore-based Dual-target Drug Profiling for Alzheimer’s Disease

P-283	Susmita Mandal	Synthesis of Thioamide Derivatives in Environmentally Benign Deep Eutectic Solvent (DES): A Green Approach
P-284	Susobhan Swain	Selective Sensing of L-Cysteine by Silver Nanogranules Incorporated RhB Nanocomposites
P-285	Svadha Devi	Pyridine-bridged Molecular Flexibility and its impact on FWHM and ΔE_{ST}
P-286	Swati Samantaray	Redox-neutral zinc-catalyzed cascade [1,4]-H shift/annulation of diaziridines with donor-acceptor aziridines
P-287	Swmkwr Brahma	Diorganotin(IV) complexes with bulky quadridentate salphen-type Schiff base (N_2O_2) incorporating diazenylpyridyl side arms
P-288	Tanaya Medhi	Synthesis, characterization and study of catalytic degradation of methyl orange by an oxidovanadium(IV) Schiff base complex derived from glycine
P-289	TanjilaBegum	One-pot facile green synthesis of ruthenium nanoparticles embedded in the nanoglobules of aloevera gel with anticancer potential
P-290	Tanushree Das	Point-of-Care Testing of Uric Acid Using Gold Nanostar Embedded Robust and Reusable Hydrogel Beads Showing Photo-Oxidase Like Activity
P-291	Tanvi Singh	Blossoms of Health: A Review of the Nutraceutical and Medicinal Properties of Indian Flowers
P-292	Tapashi Das	Selective sequential oxidation of N-substituted tetrahydroquinoline using cyclometalated ruthenium(II) complex
P-293	Thangaraj Devaraj	Synthesis of 1,2,3,4-Tetrahydroquinolines from N-Unsubstituted Aminomethyl Donor-Acceptor Cyclopropanes
P-294	Thangjam Sanjurani	Green synthesis of Schiff base containing sulphur bond and its Cu(II) complexes: Crystal structure Analysis, Hirshfield Analysis, DNA binding studies, in-vitro biological Assessment, quantum chemical calculations and Docking studies.
P-295	Thanseeha Sherin P A	Facile Fabrication of multi-functional super hydrophobic surfaces synthesized by additive manufacturing technique modified with ZnO nanoparticles
P-296	Tirtharaj chetry	GC-MS analysis of Aristolochia rathyae collected from Arunachal Pradesh, north east India.
P-297	Tohira Banoo	Investigation of Anticancer activity of self-assembled biocompatible glycoconjugates derived from Bhilawanol
P-298	Trishna Saikia	A new rhodamine isoindoline based fluorescent chemosensor for the detection of Fe (III) ions
P-299	Trishnajyoti Baishya	Supramolecular Assemblies in Dicarboxylate based Metal-Organic Co-crystal Hydrates of Mn(II), Cu(II) and Ni(II): Combined Experimental and Theoretical Studies
P-300	Uddit Narayan Hazarika	Highly conductive small in situ generated ligand-based metal organic frameworks
P-301	Vandana Vishwakarma	Synthesis of Copper MOF with carboxylic acid based ditopic linker for Efficient removal of organic dye from aqueous solution.
P-302	Vasavi S Pai	Molecular Docking and Dynamics of a Novel Inhibitor Targeting Mutant IDH1 in Cancer
P-303	Vedant Phad	On the Accuracy of ML-BOP Model in Reproducing the Properties of High-Pressure Ices
P-304	Vijesh Tomar	Iron-Catalyzed Synthesis of Ferrocenyl-thioether Conjugates via C-S Cross Coupling of Thioethers and Vinyl Chlorides: Construction, Anticancer and Computational Studies
P-305	Vishnu N. Vijayan	ε Poly L lysine: A Naturally Occurring Biodegradable Polypeptide for Selective Detection of 5 Nitroimidazole Antibiotics in Animal Products and Living Cells via Fluorescence
P-306	Wolfgang Haumer	A hydrazine-free photoredox catalytic synthesis of azines by reductive activation of readily available oxime esters
P-307	Yogendra Kumar	Regioselective Synthesis of 4-Arylamino-1,2-Naphthoquinones in Eutectogel as a Confined Reaction Media using LED Light

P-308	Yogesh Kumar Verma	Folic Acid and Cyclodextrin Functionalized Silk fibroin-capped Gold Nanoparticles for Targeted Delivery of Anticancer Drug
P-309	Namrata Kotwal	Organocatalytic Asymmetric Synthesis of Carbo- and Oxa-Cyclic Seven-Membered Bridged-Biaryls via Domino Sequence

PL-1

How to design polymers to fulfil functions in biosensors, thermoelectrics and batteries?

Mukundan Thelakkat,
Applied Functional Polymers, University of Bayreuth Bavarian Polymer Institute (BPI),
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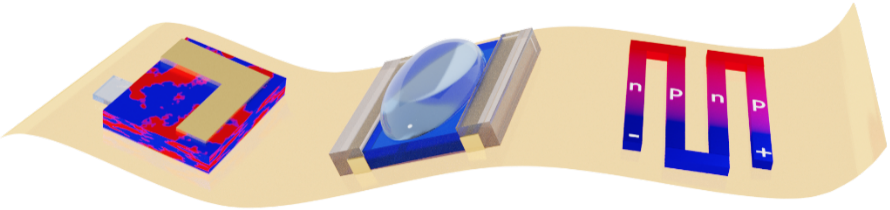

The main theme of the talk will be the principles of polymer architecture and structural changes in conjugated polymers, conjugated polyelectrolytes and polymer electrolytes to fulfil diverse properties in modern applications such as solar cells, biosensors, thermoelectrics as well as batteries. The diverse applications demand a wide variety of structural changes and adaptation of hydrophobicity and hydriophilicity in addition to tuning and optimization of charge transport from pure electronic or ionic conductors to mixed conductors. With suitable examples of polymers, the design principles and applications will be demonstrated in various devices. An additional aspect of doping of conjugated polymers and the consequences of a novel and stable p-doping strategy will also be discussed.

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2. *A competitive n-Type OECT Material via Copolymerization of Electron Deficient Building Blocks; Erhardt, MT, et al. Adv. Electron. Mater.* ***2023****, 2300026*
3. *Solid polymer electrolytes from polyesters with diester sidechains for lithium metal batteries, D. Rosenbach, M. Thelakkat et al, J. Mater. Chem. A* ***2022****, 10, 8932-8947.*
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PL-1

Brief Biography
Mukundan Thelakkat

Mukundan Thelakkat is born in a remote village, Konnencherry, Palakkad District, Kerala State, India and he studied upto Masters in Chemistry under different colleges in Calicut and Kerala Universities in Kerala. He could afford his Masters study only because of a national merit scholarship and he was first Rank holder in MSc at Calicut University, Kerala. He moved abroad with an international PhD fellowship and after obtaining PhD in Organic and Polymer Chemistry from Friedrich- Schiller University, Jena, Germany in 1992, Thelakkat joined one of the biggest multinational Chemical Companies in Germany, BASF at Ludwigshafen, as a Postdoc. In 1995, he returned to academia and joined The University of Bayreuth, Germany as a guest scientist and qualified for being a Professor by finishing *Habilitation in Polymer Chemistry and Functional Materials*. In 2004, Thelakkat had a research stay at General Electric Research (GE, New York State, USA). From 2006 onwards is Thelakkat Professor for Applied Functional Materials at The University of Bayreuth, Germany.

The key theme running through his research work is design, synthesis and applications of tailor-made functional materials for electronic and electrical applications. The main emphasis is on energy conversion and storage. The diverse device applications include organic field effect transistors, biosensors, batteries, solar cells and thermoelectrics. Most of these devices based on soft polymeric functional materials allow the fabrication of devices in non-conventional, flexible, stretchable and implantable geometries as shown in a sketch below.

Thelakkat has coordinated many international multimillion Euro research projects on energy topics, he is Board member of Bavarian-Indian Science and Technology Centre (BAYIND) in Germany, he is Advisory Board Member of Presidential Commission of Internationalization at University of Bayreuth. He is also Member of Bavarian Polymer Institute (BPI) and Bavarian Battery Technology Center (BAYBATT). At present, he is a visiting VAJRA Fellow of DST at JNCASR, Bangalore.

Scientific & Publications record: > 260 peer-reviewed papers, about 20 international patents with companies such as BASF, Siemens, GE etc.
h-index: Google Scholar: 62, WoS: 59; Citations of papers: 13 936 (GS), 12 000 (WoS)

PL-2

Functional $K_{3,3}$ (“Kuratowski”) Building Units in Materials Chemistry: Past, Present, and Future.

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The first metal-organic framework (MFU-4, Metal-organic Framework Ulm University) comprising “*Kuratowski*-type” coordination units was reported in 2009.[1] Its strictly orthogonal geometry has inspired chemists to develop a diverse range of functional materials. Owing to a combination of nano-sized cavities and ultra-narrow pores, MFU-4 features kinetic gas trapping allowing for quantum sieving of light hydrogen isotopologues,[2] or high-capacity/slow-release entrapment of noble gas atoms.[3] Gas-specific uptake rates allowed us to construct the first MOF@SAW surface acoustic wave-based sensor.[4]

In contrast to MFU-4, the isoreticular MFU-4*l*(arge) features framework-anchored metal sites resembling the iconic scorpionate complexes (Fig.1).[5] Cu^{I}-MFU-4*l* shows reversible chemisorption of O_2, N_2, and H_2 with record-breaking isosteric heats of adsorption of 32–53 kJ mol^{-1}.[6] Biomemetic generation of catalytically active $Fe^{IV}{=}O$ species in Fe-exchanged MFU-4*l* has recently been demonstrated by Hou et al.,[7] indicating the huge potential of MFU-4-type metal–organic frameworks as catalytic materials.

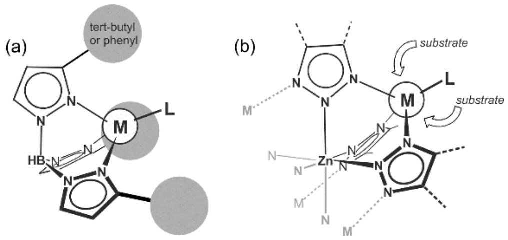

Figure 1. (a) Scorpionate complex; (b) Secondary building (“*Kuratowski*-type”) unit from MFU-4*l* comprising open metal sites. (M = transition metal, L = ligand)

Apart from the above mentioned applications, framework materials containing Kuratowski-type building units, such as simple M(II)-triazolate frameworks, often show fascinating physical properties, ranging from cooperative large-hysteresis spin-crossover in $[Fe^{II}(ta)_2]$ to spin-liquid behaviour in $[Mn^{II}(ta)_2]$, to name only a few examples.[8, 9] Research activities in our group have recently turned to photoactive metal complexes and frameworks for which the programmable self-assembly of $K_{3,3}$ units offers an efficient bottom-up approach toward artificial photoantenna systems.

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PL-2

Brief Biography
Dirk Volkmer

Dirk Volkmer obtained his Dr. of Science in Inorganic Chemistry from the University of Münster (Westphalia), Germany. He spent the academic years 1995–1996 as Feodor Lynen post-doctoral fellow at the Université Louis Pasteur (Strasbourg (France), with Prof. Jean-Marie Lehn).
During the period of 1996 – 2004 he stayed as a so-called "Habilitand" (= German academic equivalent to an Assistant Professor) at the University of Bielefeld (Germany, with Achim Müller), including a short stay from 1998–1999 at the Weizmann Institute of Science (Rehovot (Israel), with Prof. Lia Addadi), where he went as a Minerva fellow.

From 2004 – 2010 he became Associate Professor at the University of Ulm (Germany), after which he accepted his present position as Full Professor and Chair of Solid State and Materials Chemistry at the Institute of Physics, University of Augsburg (Bavaria, Germany).

His main research interests lie in coordination chemistry and in the design of biologically inspired materials, both being merged into functional porous framework materials. Applications range from sorption and gas separation, activation of small molecules, heterogeneous catalysis to sensors and nanodevices. In 2008 he received the Merckle (Ratiopharm) Award for the development of biomimetic materials.

PL-3

The Chaotropic Effect as an Assembly Motif in Chemistry

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Following up on scattered reports about interactions of conventional chaotropic ions (e.g., I^-, SCN^-, $ClO4^-$) with macrocyclic host molecules, biomolecules, and hydrophobic neutral surfaces in aqueous solution, the chaotropic effect has emerged as a generic driving force for supramolecular assembly, orthogonal to the hydrophobic effect. The chaotropic effect becomes most effective for very large ions that extend beyond the classical Hofmeister scale, and that can be referred to as superchaotropic ions (e.g., borate clusters and polyoxometalates). We present a continuous scale of water-solute interactions (Scheme below) which includes the solvation of kosmotropic, chaotropic, and hydrophobic solutes.[1] Recent examples for the soft-matter association of chaotropic anions to hydrophobic macrocyclic binding sites,[2,3] colloids,[4] lipid bilayers,[5] peptides,[6] proteins,[7] and surfaces are discussed, and a new application line will be described. Namely, we have introduced the use of superchaotropic anions as transmembrane transporters in cell biology and medicinal chemistry, including borate clusters,[5-8] metallacarborane ions,[9] and polyoxometalates.[10]

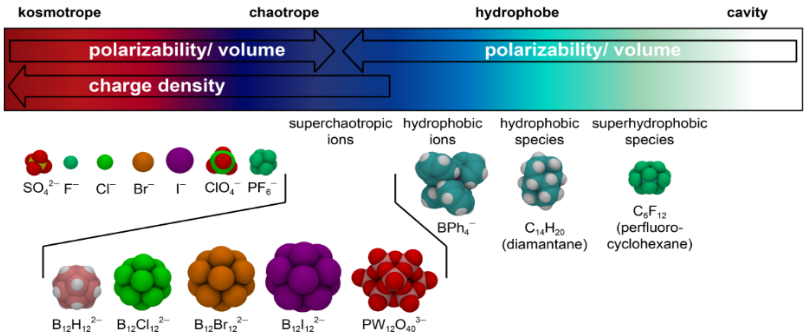

Figure 1. Continuous scale for hydration of different species in water

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PL-3

Brief Biography
Werner M. Nau

Profile

1994 Ph.D. in Physical Organic Chemistry at the University of Würzburg, Germany
1994–1995 Postdoc at University of Ottawa, Canada
1996–2002 Assistant Professor at the University of Basel, Switzerland
2002–today Professor of Chemistry at Constructor University, Germany
2012–2023 Dean of Science at Constructor University, Germany
2023–today Vice President for Academic Operations at Constructor University, Germany

Research Summary

Our research combines principles of organic photochemistry with spectroscopy and supramolecular chemistry and is directed towards applications in bioanalytical chemistry, peptide folding, drug delivery, drug discovery, catalysis, chiral recognition, fluorescent dye design, chemosensing, as well as enzyme and membrane assays. Our group is known for the description of high-energy water as contributor to assembly processes in aqueous solution (Isr. J. Chem. 2011, 51, 559; JACS 2012, 134, 15318; ACIE 2014, 53, 11158; > 1650 citations) and for the introduction of the chaotropic effect as a complementary driving force to the hydrophobic effect (ACIE 2015, 54, 6852; ACIE 2018, 57, 13968; >600 citations). We have pioneered time-resolved variants of indicator displacement assays known as supramolecular tandem enzyme/membrane assays (Nat. Meth. 2007, 4, 629; Chem. Rev. 2011, 111, 7941; Chem. Eur.J. 2012, 18, 3444; Acc. Chem. Res. 2014, 47, 2150; Adv. Mater. 2024, 36, 2306922; > 2000 citations). Our work on fluorescent sensors, macrocycles, and particularly cucurbiturils (JACS 2004, 126, 5806; Chem. Soc. Rev. 2015, 44, 394; >1900 citations), high-affinity binders (including, most recently, boron clusters) and complexation-induced pKa shifts (Adv. Drug Del. Rev. 2012, 64, 764) has found applications in pharmaceutical drug discovery and drug delivery, exemplified by the most recent discovery of a new class of transmembrane carriers together with Javier Montenegro (see abstract).

Bibliometric Data

We have written more than 300 original research publications, more than 100 of which in top multidisciplinary journals, such as Nature, Nat. Chem., Nat. Meth., Proc. Natl. Acad. Sci. U.S.A.,

J. Am. Chem. Soc., Angew. Chem., Adv. Mater., etc.; additionally 8 book chapters and 4 patents.

- ca. 24000 citations (since 1993), citation average per peer-reviewed publication: > 75
- h-index 78 (age: 56)

KL-1

New Concepts in Visible Light-Powered Catalysis: Organophotocatalytic Dyads and Autophotocatalysis

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In this talk, two new concepts in visible light-powered catalysis will be presented: **Topic 1: organophotocatalytic dyads:** Molecular organic dyads consisting of linked Donor-Acceptor (D-A) moieties find numerous applications as optical and light-harvesting devices.[1] Photoexcitation leads to charge separated (CS) states, that can be advantageous or parasitic depending on the target application. Building on previous learnings on pre-assembling electrogenerated radical cationic and anionic photocatalysts pioneered by our group,[2] this talk exemplifies how CS states pre-assemble electronically-complementary reaction partner substrates (Figure 1, top). Upon photoexcitation of the resulting CS state-substrate complex, transient radicals – that would otherwise undergo deleterious defunctionalizations / polymerizations – are generated and react selectively in close proximity for useful cross-couplings. This demonstrates a conceptual metal-free alternative to transition metal catalysis for intercepting transient radicals, and demonstrates the key importance of aggregation in photochemistry, often overlooked by synthetic chemists. **Topic 2: photoredox autocatalysis:** Sulfonamides and biaryls are relevant in medicinal chemistry and ubiquitous in pharmaceuticals. Cyclic biaryl sulfonamides (**BASN**s) are emerging bioactive motifs with anticancer potential.[3] This talk reports a novel 'auto'-photoredox catalysis (auto-PRC) pathway to **BASN**s, an efficient process where the product itself acts as a photocatalyst[4] (Figure 1, bottom). We exemplify the power of auto-PRC in photocatalyst library construction and screening, identifying potent reductive photocatalysts applied to diverse organoradical precursors (60 synthetic transformations). Both topics are scalable to grams in flow.

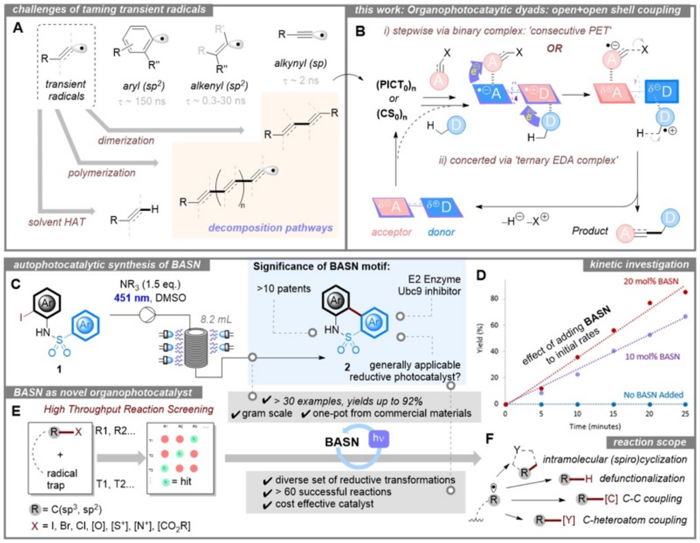

Figure 1. Top, **topic 1**: challenges of transient radicals (A), concept of organophotocatalytic dyads (B). Bottom, **topic 2**: autophotocatalytic synthesis and significance of **BASN**s (C), kinetic investigations (D), high throughput screening concept (E) and diverse scope of reactivity (F).

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KL-1

Brief Biography

Joshua P. Barham

Dr. Joshua P. Barham is a Reader at the University of Strathclyde, UK, and an Adjunct Professor at Universität Regensburg, Germany. A rising star in the field of organic chemistry, he has raised over €3.9 million since starting his independent research career in December 2019. His research spans synthetic photoelectrochemistry, photocatalysis, continuous flow chemistry, and automation. His work is widely recognized, with 39 publications, including four ESI Highly Cited Papers, ten journal covers, and two patents, alongside over 2,150 citations (h-index: 23, i10-index: 33).

Dr. Barham holds a Ph.D. in Organic Chemistry from the University of Strathclyde, completed in collaboration with GlaxoSmithKline, and an MSci with First-Class Honors from University College London. He further honed his expertise during postdoctoral fellowships in Japan under the prestigious JSPS and NEDO programs.

His career highlights include prestigious awards such as the ERC Starting Grant (2022), the Sofja Kovalevskaja Award from the Alexander von Humboldt Foundation (2019), and selection as one of 14 young academics worldwide for the SCS Bürgenstock Conference (2024). He was also a Reaxys PhD Prize Winner (2017) and received the Silver Award at the UK Parliament's "SET for Britain" competition (2016).

Dr. Barham is an invited speaker at over 30 international conferences and a regular peer reviewer for leading journals such as *Nature Catalysis*, *JACS*, and *Angewandte Chemie*. He is an active member of multiple esteemed societies, including the Royal Society of Chemistry, ACS, GDCh, and the DFG Collaborative Research Centers.

Currently leading groundbreaking research at the intersection of photochemistry, catalysis, and automation, Dr. Barham is a leading voice shaping the future of sustainable organic synthesis.

KL-2

Scanning Probe Lithography for Precision Chemical Surface Engineering and Device Functionalization

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Scanning probe lithography (SPL) techniques, including dip-pen nanolithography (DPN), polymer pen lithography (PPL), and microchannel cantilever spotting (μCS), present powerful tools for localized chemical surface functionalization with high precision, offering spatial resolutions from the micron down to the nanometer scale.[1] Each method offers unique advantages in terms of resolution, throughput, and patterning speed, while maintaining broad compatibility with delicate chemical and biological inks. Importantly, these techniques are characterized by mild process conditions, preserving the functionality of sensitive compounds and facilitating multiplexed deposition of various materials within complex micropatterns. This versatility makes SPL techniques particularly attractive for creating bioactive surfaces and biohybrid devices, where traditional and biological materials converge for biomedical applications. In addition to biohybrid devices, SPL is highly relevant in biomaterials research, enabling the fabrication of patterned substrates that can be used to study cell-surface interactions in detail. SPL's potential for combining functional materials at the nanoscale opens doors to innovations in biosensing, tissue engineering, and drug delivery systems. As a precise, adaptable, and scalable lithography platform, SPL enables the integration of complex chemical architectures onto surfaces, paving the way for next-generation biomedical devices and novel therapeutic approaches.

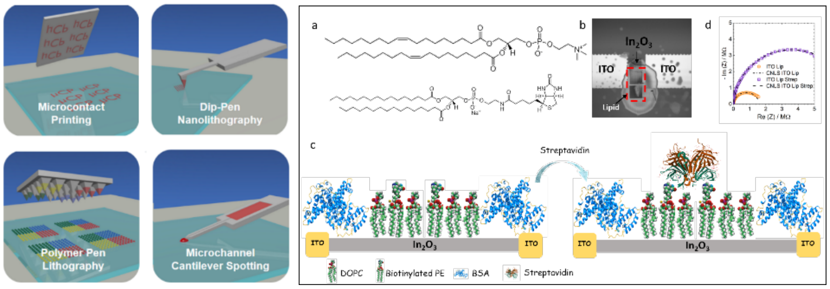

Figure 1. Schematic depiction of some scanning probe lithography methods (left) and example of a bio-hybrid device, combining an electronic device with a biomimetic lipid membrane functionalization (right).

In my talk, I will present selected examples from our works and collaborations on applications of SPL for biosensor immobilization,[2] biomedical diagnosis platforms,[3] and the microscale tuning of surface wettability.[4,5] New results on biomimetic lipid membranes as component of an electronic device, read-out via electrochemical impedance spectroscopy (EIS) for sensitive protein detection will exemplify the potential of SPL for biohybrid sensor devices.

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KL-2

Brief Biography
Michael Hirtz

PD Dr. Dr. Michael Hirtz

Institute of Nanotechnology (INT) and Karlsruhe Nano Micro Facility (KNMFi)
Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Michael Hirtz is leader of the group for “Scanning Probe Lithography for Biomaterials and Bioelectronics” situated in the research unit of Prof. Aghassi-Hagmann at the Institute of Nanotechnology (INT) of the Karlsruhe Institute of Technology (KIT), Germany. He holds a PhD in physics and in medical sciences from the University of Münster. After doing research on self-organization phenomena in phospholipid films generated by Langmuir-Blodgett technique during his PhD, he is now focusing on advancing Dip-Pen Nanolithography and other Scanning Probe Lithography methods for applications at the interface of physics, surface chemistry and biomedical applications. In 2018, he received the "High-End Foreign Talent" of Shanxi Province, China and recently became Honorary Faculty member at the Centre for Nanotechnology at IIT Guwahati, India (2021).

For an overview of his work and publications please visit:
https://www.researchgate.net/profile/Michael_Hirtz
https://www.webofscience.com/wos/author/rid/C-8821-2011
http://scholar.google.de/citations?user=Wy00YA4AAAAJ

Or have a look at his group home page:
http://www.int.kit.edu/900.php

KL-3

Solar Fuel Production through Post-Synthetic Modification of Metal-Organic Frameworks

Tapas K Maji

Molecular Materials Laboratory, Chemistry and Physics of Materials Unit, School of Advanced Materials (SAMat),
Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur Post, Bangalore- 560064, India.

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The much-needed renewable alternatives to fossil fuels can be achieved efficiently and sustainably by converting solar energy to fuels via hydrogen generation from water or CO_2 reduction. Sunlight-driven H_2 production and CO_2 reduction are promising routes for the production of chemical feedstocks as fuel precursors to mitigate the CO_2 concentration in the atmosphere and also to alleviate the global energy crisis. [1-5] Nature's design of carrying out the photosynthetic redox cycle involving CO_2 and water inspired us to develop highly efficient integrated catalytic systems for artificial photosynthesis. The versatile and highly amenable structural tunability of metal-organic frameworks (MOFs) by post-synthetic modification (PSM) allows for tailoring inherent semiconducting and optoelectronic properties, compared to traditional inorganic semiconductors. Besides, PSM is an excellent choice for introducing a functional photosensitizer into the MOF matrices to galvanize the electronic and optical properties towards photocatalytic H_2O and CO_2 reduction. [1-3] Our presented results demonstrated an excellent approach to green H_2 production and carbon neutralization for tackling the energy crisis. [1-6]

My talk will focus on developing integrated photocatalytic systems through post-synthetic modification of MOFs for H_2O and CO_2 reduction.

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KL-3

Brief Biography

Tapas K Maji

Prof. Tapas K. Maji's research centers on the synthesis and structure-property relationships of metal-organic frameworks (MOFs) and porous organic polymers (POPs) at both bulk and nanoscale levels. He has made seminal contributions to MOF and POP research, demonstrating their diverse applications, including cost-effective chemical feedstock separation, geometrical isomer separation, and the removal of toxic metal ions from water. In a pioneering approach, he developed a method of covalently linking light-harvesting units with catalytic moieties in MOFs, opening new avenues for creating artificial photocatalysts for clean solar fuel production. To further enhance the versatility of these hybrid materials, Prof. Maji's team developed 'soft' gel materials by self-assembling low molecular weight gelators (LMWG) with metal ions, which have applications in catalysis and optoelectronics.

Dr. Maji received the Shanti Swarup Bhatnagar (SSB) Award in Chemical Sciences (2019). He is also recipient of several other recognitions such as Bronze Medal of the Chemical Research Society of India (CRSI) & Materials Research Society of India (MRSI), the Sheikh Saqr Career Award Fellowship from JNCASR, and the Scopus Young Scientist Award, Senior AvH Fellowship (Germany). He is a Fellow of the Royal Society of Chemistry (RSC) recognized as a Leader in the Field in 2019, and the Indian Academy of Sciences.

KL-4

Are there sugars in bacteria? What can we do with them?

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Bacterial glycoconjugates are comprised of rare D and L deoxy amino sugars, which are not present on the human cell surface. This peculiar structural difference allows discrimination between the pathogen and the host cell and offers avenues for target-specific drug discovery and carbohydrate-based vaccine development.[1] However, they cannot be isolated with sufficient purity in acceptable amounts, and therefore chemical synthesis is a crucial step toward the development of these products.[2,3] We recently established short and convenient methodologies for the synthesis of orthogonally protected bacterial D and L-deoxy amino hexopyranoside and glycosamine building blocks starting from cheaply available D-mannose and L-rhamnose.[4,5] The one-pot protocols rely on highly regioselective nucleophilic displacements of triflates. These procedures have been applied to the synthesis of various bacterial glycoconjugates[6] as well as metabolic oligosaccharide engineering.[7] The studies led to discovery of selective inhibitors of glycan biosynthesis.[8]

In this talk I will present our recent results on the total synthesis of highly complex and densely functionalized glycoconjugates and the application of rare sugars in selective detection and disarming of pathogens as well as vaccine development.

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KL-4

Brief Biography

Suvarn Kulkarni

Suvarn Kulkarni received his Ph.D. in Organic Chemistry from University of Pune in 2001. After his Ph. D., he pursued his post-doctoral research at Academia Sinica, Taipei, and University of California, Davis. He returned to India in late 2008 and held a faculty position at IACS Kolkata prior to joining the Indian Institute of Technology Bombay in 2009. He is presently working as Biswas-Palepu Distinguished Chair Professor and Dean of Academic Programs at IIT Bombay. His current research interests include devising newer ways for efficient chemical synthesis of rare sugar containing complex glycoconjugates specifically expressed on the surfaces of pathogenic bacteria for the development of antibiotics, therapeutics and vaccines.

Suvarn was a short term Visiting Professor (MOST) at Taiwan in 2014. He is a Fellow of the Royal Society of Chemistry London, Fellow of National Academy of Science (NASI) and Fellow of Maharashtra Academy of Science. He is a recipient of the CRSI Bronze medal for the year 2017 and Dr. H. C. Srivastava Young Scientist award 2016. He is a member of the editorial board of Carbohydrate Research and guest editor of international journals such as EJOC, OBC and Frontiers in Chemistry. Recently he received IRCC research Dissemination Award and Research Publication Award from IITB. Most importantly, he was selected by the students for the Excellence in Teaching Award at IIT Bombay in 2017 and also for the prestigious Prof. S. P. Sukhatme Award for Excellence in Teaching in 2020.

IL-1

Can Visible Light Do Selective Dearomative C-H Activation

Debayan Sarkar*
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Aromatic hydrocarbons are the economic class of feedstock which are available in plenty all around. Generation of multi-functional three-dimensional structures from these simple planner aromatic compounds allow a fast access to solve complexity at higher levels. The focal point lies on the fact, that a wide range of carbon-carbon and carbon-heteroatom bond formations are possible with this key transformation. Specially, the CADR's developed by You. *et. al.* has attracted a world-wide attention. Transition metal complexes based on Os, Ru, Re, Cr, Mn etc. in stoichiometric amounts have shown predominance in these transformations, the toxicity and cost related to the use of these complexes behave as deterrents of their ample use in synthesis. The exhaustive resonance stabilization renders arenes particularly unreactive as starting materials. Protocols which can circumvent this inertness are scanty. This inertness often leads to side reactions like dimerization and decomposition of the substrate. Notable contribution from our lab includes the tribromides as key resource of dearomatization. Our perruthenate generated catalyzed *ipso*-dearomative spiro-etherification and spiro-amidation of phenols delivers an insight catalytic dearomative spirocyclisation. Albeit, we envisioned that a photocatalytic oxidation of phenols with visible light in presence of aerial oxygen as oxidant would be a certain advancement of dearomative chemistry.

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IL-1

Brief Biography

Debayan Sarkar

Dr. Debayan Sarkar is presently an Associate Professor of Chemistry at the Indian Institute of Technology Indore (IIT Indore). Before this he worked as an Associate Professor in the Department of Chemistry at National Institute of Technology, Rourkela, Odisha, India. He has completed his M.Sc with Organic Chemistry 32pecialization from University of North Bengal (NBU) in the year 2005 followed by a Ph.D in Organic Synthesis from Indian Association For The Cultivation of Science (IACS) in the year 2011, Jadavpur Kolkata under the supervision of Prof. R. V.Venkateswaran in 2011. After that he travelled to carry out his post-doctoral studies at Stanford University (USA) under the mentorship of Prof. Barry M Trost (2012-2013). He was recently deputed as a Visiting Senior Assistant Professor at Graduate School of Pharmaceutical Sciences, Tohoku University (Japan) under the mentorship of Prof. M. Yamaguchi (2015- 2016). He was at the University of Leipzig Germany as a DAAD Research Professor with Prof. Christoph Schneider (2018-2019). He worked with Prof. Burkhard Koenig at University of Regensburg Germany as an ICMR International Fellow from Jan-Dec 2020. He has been recipient of prestigious awards like Chemcomm Pioneering Investigators 2024, IIT Indore Best Research Paper award 2024,SERB TETRA Award, RC Tripathy Research Excellence Award by Orissa Chemical Society, DST Inspire faculty award (2013),BRNS-DAE Young Scientist Award (2014), Indo-US Research Award(2012), DAAD Visiting Professor (2018). Research interest includes Visible Light Catalysis, Asymmetric Dearomatisation reactions, Atom Economic couplings, Complex total synthesis of natural products. He has 65 research publications in International Journals of Repute, 2 Patents and guided 8 Ph.D students and 12 Ph.d students are presently undergoing their doctoral studies under his supervision. Presently, he is also heading the Centre for Rural Development and Technology (CRDT) at IIT Indore.

IL-2

Regulating Chemo- and Regio-selectivity through Controlled Electrolysis

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Mohanpur-741246, West Bengal, India
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Chemoselectivity is a critical concept in organic synthesis, where precise control over the reactions occurring at different functional groups is essential.[1] In the first part of the talk, a regio-divergent synthetic approach to access highly substituted indole scaffolds will be illustrated. The developed tuneable electrochemical strategy exploits two analogous styrylaniline precursors and permits nice control on the chemoselectivity over the C-3 substitution pattern, governed by the acidity of the amide proton.[2] A follow-up formal [3+2] cycloaddition strategy between *α*-amino carbonyls and tosylmethyl isocyanide (TosMIC) will be depicted, permitting the fabrication of 1,5-disubstituted imidazole derivatives.[3] Next, an electrochemical heterocoupling between two *N*-aryl glycinate derivatives will be presented, which provides highly stereoselective 4,5-dihydro-1*H*-imidazole carboxylates.

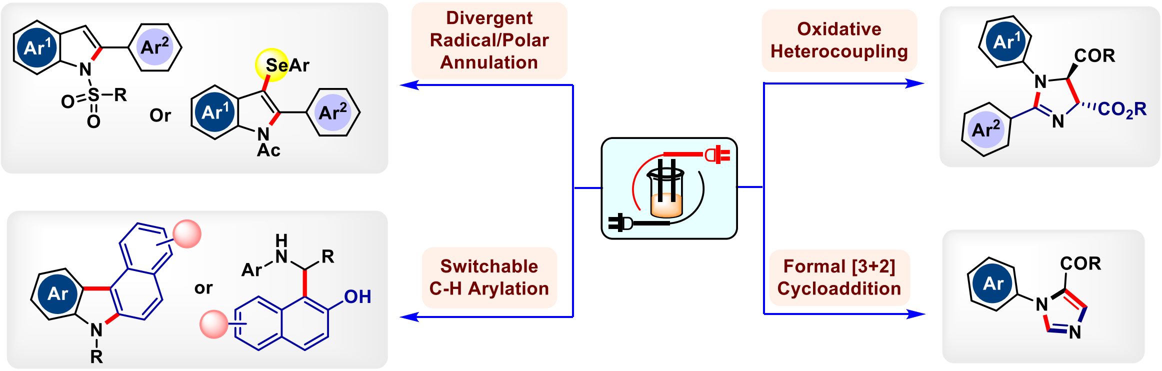

Figure 1. Chemo- and regio-selective synthesis of various heterocycles through controlled electrolysis

Finally, a switchable regioselective C(sp^2)-H/C(sp^3)-H arylation leading to highly substituted carbazole manifolds or substituted glycinate derivatives will be demonstrated.[4]

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IL-2

Brief Biography

Suman De Sarkar

Suman De Sarkar received B.Sc. (2005) and M.Sc. (2007) degrees in Chemistry from University of Calcutta and IIT Kanpur, respectively. He obtained his Ph.D. in November 2010 from University of Muenster under the supervision of Prof. Armido Studer. Afterward, he worked as a postdoctoral researcher in the research group of Prof. Karl Gademann at the University of Basel (2011-2013) and with Prof. Lutz Ackermann as an Alexander von Humboldt Postdoctoral Fellow at the University of Goettingen (2013-2015). In October 2015 he joined IISER Kolkata, as an Assistant Professor and in September 2019 was promoted to the post of Associate Professor. His research interests are the application of redox-mediated transformations in organic synthesis with a special focus on electrochemistry and photocatalysis.

Selected Publications:

1. T. Mandal, S. Mallick, M. Islam, **S. De Sarkar***, *ACS Catal.* **2024**, *14*, 13451.
2. S. K. Saha, S. Mallick, A. Nath, **S. De Sarkar***, *Org. Lett.* **2024**, *26*, 7330.
3. M. Baidya, D. Maiti, L. Roy*, **S. De Sarkar***, *Angew. Chem., Int. Ed.* **2022**, *61*, e202111679.
4. D. Maiti, K. Mahanty, **S. De Sarkar***, *Org. Lett.* **2021**, *23*, 1742.
5. **S. De Sarkar***, *Angew. Chem., Int. Ed.* **2016**, *55*, 10558.

Awards/Achievements:

- CRSI Bronze Medal **2025** (Announced)
- Editorial Board member of Tetrahedron & Tetrahedron Letters **2024**
- Member of the Early Career Advisory Board of Asian Journal of Organic Chemistry
- Thieme Chemistry Journals Award 2023
- Fellow of the Indian Chemical Society
- DSM Science & Technology Award, Netherlands (**2011**)
- D. C. Mukherjee Gold Medal award (**2005**)

IL-3

Exploiting α-Gem-Boryl Carbanions and Vinyl Boronates for Diverse Synthetic Applications

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Indian Institute of Technology Kharagpur
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Zweifel olefination is an attractive transition metal-free method for the stereoselective synthesis of olefin. Although several developments have been made in the Zweifel olefination and its extension to heterocyclic synthesis, the chemistry remains mostly reserved either between a pi-inactive and pi-active system or using similar olefin on both sides to control the stereoselectivity. The reactivity between two unsymmetrical olefins or between a heteroaryl and vinyl boronates is mostly unknown, which undermines its scope and impacts on organic synthesis. We have developed a stereoselective 1,2-migration from a substituted vinyl and heteroaryl boronate complex, which has produced cis-or trans-vinyl heteroaryl, an important skeleton present in bioactive compounds and natural products. Geminal bis(boron) compounds have recently emerged as valuable building blocks for the synthesis of molecules with structural diversity. They have the advantages of unique stability, and operational simplicity and can be engaged in several kinds of transformations. The easy generation of α-bis(boryl)organometallic species from the corresponding geminal-bis-boron compounds allows diverse synthetic transformations. We have applied this concept for the synthesis of enyne MIDA boronates and one pot conversion of phenol to benzaldehyde.

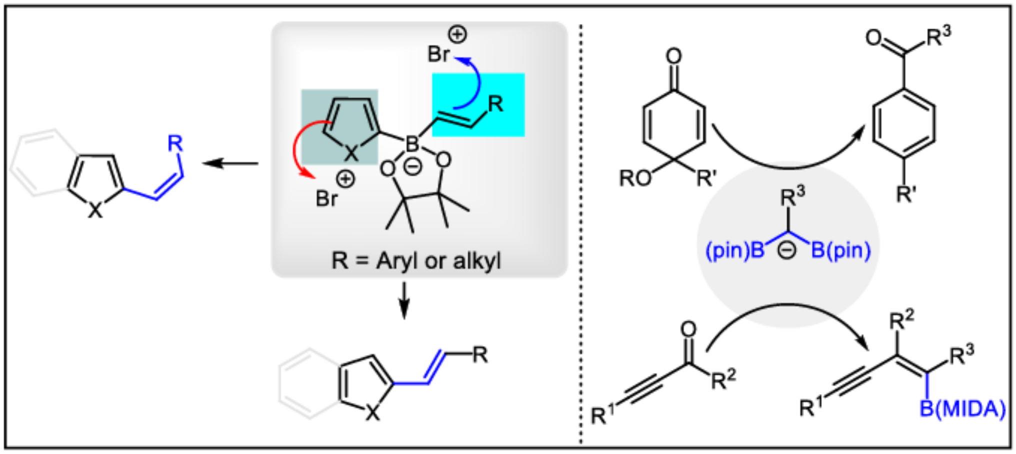

Figure 1. Exploiting α-Gem-Boryl Carbanions and Vinyl Boronates for Diverse Synthetic Applications

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IL-3

Brief Biography

Santanu Panda

Dr. Santanu Panda obtained his PhD on 2013 in organocatalysis and total synthesis of natural products under Prof. Antony Pearson, Case Western Reserve University, Cleveland, USA. After finishing his PhD, he moved to Dallas and joined Prof. Joseph Ready group as postdoc. During his postdoc, he was exposed to transition metal catalysed cross coupling and organoboron chemistry. On July 2018, he joined IIT Kharagpur as an assistant professor. His group is very much active in organoboron chemistry, total synthesis of natural product and organophotoredox chemistry.

Awards / Honors / Membership:

- 2023 Merck Young Scientist award, Winer.
- 2022 CRS (Chirantan Rasayan Sanstha) Bronze Medal
- 2018 Ramanujan Fellowship from SERB
- Best Poster Award at UTSW Biochemistry Retreat at Dallas Botanical Garden, Dallas On 2017.
- Invited seminar to the annual UTSW Biochemistry department seminar series at UT Southwestern Medical Center, Dallas.
- Graduate outstanding teaching assistant award 2013, Department of Chemistry, Case Western Reserve University, USA.

Representative Publications:

Org. Lett. 2024, 26, 6760
Org. Chem. Front., 2024, 11, 854
Nature Commun., 2024, 15, 3794
Chem. Sci., 2024, 15, 4989
Chem. Asian J. 2024, 19, e202300911
Chem. Eur. J. 2024, 30, e202303056
Chem. Commun., 2023, 59, 14447
Org. Lett. 2023, 25, 314-319
Angew. Chem. Int. Ed., 2023, DOI: 10.1002/anie.202309136

IL-4

Cu(I)-Catalyzed Enantioselective Hydrocupration

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Enantiomerically enriched complex alcohols are presented in wide range of small molecule therapeutics and biologically active natural polyketides. Therefore, exploring the general methods for the enantioselective synthesis of substituted alcohols is an attractive target in organic synthesis. Here, we have developed the Cu(I)-catalyzed enantioselective hydrocupration[1-2] for the synthesis of complex 1,2-*syn-sec,tert*-diols, α-hydroxy allyl ketones and propargyl alcohols using reductive coupling of carbon-carbon π-bonds with carbonyl compounds.

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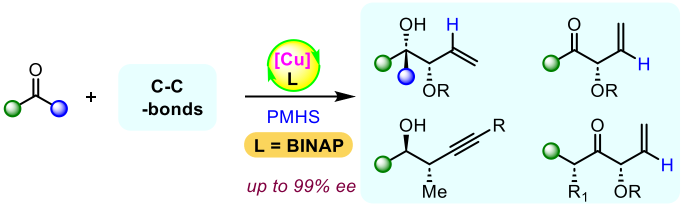

Figure 1. Enantioselective hydrocupration to access chiral alcohols

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IL-4

Brief Biography
Rambabu Chegondi

Rambabu Chegondi received his M.Sc. (2003) degree from University of Hyderabad and completed Ph.D. (2009) in Organic Synthesis from Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad under the supervision of Dr. S. Chandrasekhar. In 2009, he moved to The University of Kansas, USA to work with Prof. Paul R. Hanson as a postdoctoral researcher. He joined CSIR-IICT, Hyderabad as CSIR-Pool-Scientist (SRA) in 2014 as an independent researcher. He is currently a Principal Scientist at the OS&PC department, CSIR-IICT, focusing on the development of new enantioselective desymmetrization methodologies and new process development of key APIs. He has received the Eli Lilly Asia Best Thesis Award 2009, AVRA-Young Scientist Award-2019, Thieme Chemistry Journals Award, and SERB-STAR Award. He is an FRSC and currently an Editorial Advisory Board Member of Organic Letters.

Representative publications:

1. Jadhav, S. B.; Dash, S. R.; Maurya, S.; Nanubolu, J. B.; Vanka, K.; Chegondi, R. *Nat. Commun.* **2022**, *13*, 854.
2. Gollapelli, K. K.; Patil, V. B.; Vinaykumar, A.; Chegondi, R. *Chem. Sci.* **2021**, *12*, 1544.
3. Thopate, S.B.; Jadhav, S.B.; Nanubolu, J. B.; Chegondi, R. *ACS Catal.* **2019**, *9*, 10012.
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IL-5

Selective Methane Oxidation to Methanol or Acetic Acid using O_2 over Metal-Organic Framework Supported Abundant Metal Catalysts

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The direct oxidation of methane to valuable oxygenates, such as alcohols and acetic acid, under mild conditions is highly challenging due to high C–H bond dissociation energy, facile overoxidation to CO and CO_2 and the intricacy of C−H activation/C−C coupling. To address this challenge, we have developed multifunctional earth-abundant metal species confined within the porous metal-organic frameworks (MOFs) for direct methane oxidation into methanol or acetic acid selectively at different reaction conditions using O_2. The heterogeneous MOF-supported single-site copper(II) hydroxyl catalyst gives exceptionally high acetic acid productivity of 1,57,366 $\mu mol_{CH_3CO_2H}\ g_{Cu}^{-1}\ h^{-1}$ in 100% selectivity at 115 °C in water. Additionally, monomeric $Fe^{III}(OH)_2$ species at the MOF nodes yields methanol or acetic acid with high productivities of 38,592 $\mu mol_{CH_3OH}\ g_{Fe}^{-1}\ h^{-1}$ and 81,043 $\mu mol_{CH_3CO_2H}\ g_{Fe}^{-1}\ h^{-1}$, respectively. The detailed mechanism of methane to methanol and acetic acid transformation will also be discussed in this talk. Through spectroscopic analyses, controlled experiments and computational studies, we demonstrate that the active-site isolation of mononuclear metal-hydroxyl species at the MOF nodes, their confinement within the porous framework, and their electron-deficient nature facilitate methane C–H activation via σ-bond metathesis, leading to the formation of methanol or acetic acid in excellent selectivity. Our rational design of MOF-based molecular base-metal catalysts and the reaction mechanism offers the development of a sustainable route for methane valorization and to synthesize methanol and acetic acid using only methane, O_2 and H_2O in a single-step without relying on precious metals, toxic CO and energy and capital-intensive syngas route.

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4. Antil, N.; Chauhan, M.; Akhtar, N.; Newar, R.; Begum, W.; Malik, J.; Manna, K. *ACS Catal.* **2022,** *12* (18), 11159-11168.

IL-5

Brief Biography

Kuntal Manna

Dr. Debabrata Mukherjee, currently serving as an Associate Professor in the Department of Chemistry at the Indian Institute of Technology Delhi (IITD), has established a distinguished academic career in inorganic chemistry and materials science. He completed his Ph.D. in Inorganic Chemistry from Iowa State University under Prof. Aaron D. Sadow, where his research focused on transition metal complexes of oxazolinylboranes and cyclopentadienyl-bis(oxazolinyl)borates as catalysts for asymmetric olefin hydroamination and acceptorless alcohol decarbonylation. Prior to this, he earned his M.Sc. in Chemistry from IIT Kanpur under the guidance of Prof. Vadapalli Chandrasekhar. His professional journey includes a significant postdoctoral research position at The University of Chicago (2013-2016) under Prof. Wenbin Lin, followed by his appointment as Assistant Professor at IIT Delhi in January 2017, where he was later promoted to Associate Professor in April 2022. Dr. Mukherjee's current research focuses on developing porous functional materials for catalytic conversion of methane, natural gas liquids (NGL), and CO2 to value-added products, engineering metal-organic framework catalysts for waste transformation, developing chiral MOFs for sustainable asymmetric catalysis, and creating organometallic complexes and nanomaterials for targeted drug delivery and biosensing applications.

AWARDS AND HONORS

- Emerging Investigators, Chemical Communications, RSC
- Early Career: Mrs. Veena Arora Faculty Research Award, IIT Delhi
- EurJIC Talents, Chemistry Europe
- Emerging Investigators, Catalysis Science & Technology, RSC
- Early Career Chemist Grant, Pacifichem, USA
- Harvinder Singh Sawhney Young Faculty Incentive Fellowship, IIT Delhi
- The Henry Gilman Fellowship, Iowa State University
- The Frank J. Moore and Thoreen Beth Moore Fellowship, Iowa State University
- Graduate and Professional Student Senate Peer Research Award, Iowa State University
- Joint Admission Test for M.Sc. (JAM) for admission to IITs: all India rank 20
- ‘First Class First’ in B.Sc. (Honours in Chemistry), Vidyasagar University, W.B., India
- Pitambar Das Memorial Scholarship with silver medal, Banamalichatta High School, India

SELECTED PUBLICATIONS (Total publications: 45, Patents: 15)

- Rahul Kalita, Manav Chauhan, Poorvi Gupta, Wahida Begum, Kuntal Manna,* Angew. Chem. Int. Ed. 2024, Accepted Article.
- Manav Chauhan, Bharti Rana, Poorvi Gupta, Rahul Kalita, Chhaya Thadhani, Kuntal Manna,* Nature Communications, 2024, in press.
- Wahida Begum, Manav Chauhan, Rahul Kalita, Poorvi Gupta, Naved Akhtar, Neha Antil, Rajashree Newar, Kuntal Manna,* ACS Catalysis, 2024, 14, 10427-10436.
- Manav Chauhan, Neha Antil, Bharti Rana, Naved Akhtar, Chhaya Thadhani, Wahida Begum, Kuntal Manna,* JACS Au, 2023, 3, 3473-3484.
- Neha Antil, Manav Chauhan, Naved Akhtar, Rahul Kalita, Kuntal Manna,* J. Am. Chem. Soc. 2023, 145, 6156-6165.
- Neha Antil, Manav Chauhan, Naved Akhtar, Rajashree Newar, Wahida Begum, Jaideep Malik, Kuntal Manna,* ACS Catalysis, 2022, 12, 11159-11168.
- Neha Antil, Naved Akhtar, Rajashree Newar, Wahida Begum, Ajay Kumar, Manav Chauhan, Kuntal Manna,* ACS Catalysis, 2021, 11, 10450-10459.
- Neha Antil, Ajay Kumar, Naved Akhtar, Rajashree Newar, Wahida Begum, Ashutosh Dwivedi, Kuntal Manna,* ACS Catalysis, 2021, 11, 3943-3957.
- Rajashree Newar, Naved Akhtar, Neha Antil, Ajay Kumar, Sakshi Shukla, Wahida Begum, Kuntal Manna,* Angew. Chem. Int. Ed. 2021, 60, 10964-10970.

IL-6

Comparing the Electronic Structure and Proton-Coupled Electron Transfer Reactivities of Cu^{III} and Ni^{III} complexes of Bis-Amidate-Bis-Alkoxide Ligands

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High-valent Cu^{III} species are frequently invoked as the key oxidants in different synthetic reactions, which include C–C, C–heteroatom bond formation, C–H bond hydroxylation, etc. However, the involvement of the Cu^{III} in the biological system is not evident. Cu-dependent monoxyganes, however, deploy the Cu^{II}/Cu^{I} redox couple for activating strong C–H bonds of substrates, which include methane, polysaccharides, glycine, etc.[1] Nevertheless, the spectroscopic identification and reactivity studies of high-valent Cu complexes are a burgeoning research interest. Ni^{III} species, which is one electron-deficient than Cu^{III}, is also frequently described as the key intermediate in versatile oxidative transformation reactions. Therefore, we set out to compare the electronic structure and proton-coupled electron transfer (PCET) studies of Cu^{III} vs Ni^{III} complexes.

We prepared the Cu^{II} (**1**) and Ni^{II} (**2**) complexes supported by electron-rich bis-amidate-bis-alkoxide ligands. The one-electron oxidation reaction of the species resulted in the formation of the Cu^{III} (**1a**) and Ni^{III} (**2a**) complexes, which were characterized by an array of spectroscopic techniques, including X-ray structure determination, X-ray absorption spectroscopy, EPR, NMR, UV-vis and cyclic voltammetry studies.[2-4] Both species revealed a significant cathodic shift of the M^{III}/M^{II} reduction potential (M = Cu/Ni). The PCET reactivity studies of **1a** and **2a** were compared toward activating the phenolic O–H bond, and the study enlightens the nature of the PCET pathway involved for both species. Further, we employed different ligand architectures, such as bis-amidate-dioxime and bis-pyridine-dioxime scaffolds, to prepare the high-valent Cu/Ni species. Although the former ligand supports the formation of M^{III} species, the latter caused the oxidation at the ligand scaffold, resulting in the generation of an iminoxyl radical species.[5] All these species were further interrogated by various spectroscopic techniques, and their PCET and ET studies have been examined.

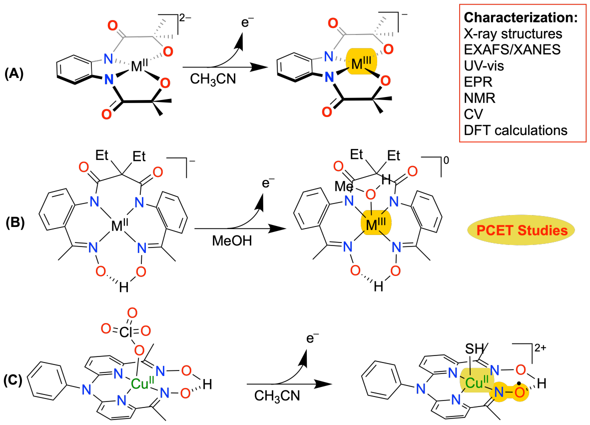

Figure 1. Structural description of the Cu and Ni complexes studied here.

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IL-6

Brief Biography

Sayantan Paria

Experience

Department of Chemistry, Indian Institute of Technology Delhi: Associate Professor, December 2022 to Present; Assistant Professor, April 2017 to December 2022. ICIQ – Institut Català d'Investigació Química, Spain: Postdoctoral Fellow, from May 2016 to March 2017. Graduate School of Engineering, Osaka University, Japan: Postdoctoral Fellow, April 2013 to April 2016.

Education

Indian Association for the Cultivation of Science, India: Ph.D, Inorganic Chemistry, 2012
IIT Roorkee, India: Master of Science (M. Sc) in Chemistry, 2007.
Vidyasagar University: Bachelor of Science (B.Sc.) in Chemistry Honors, 2005.

Fellowship and Awards

- Postdoctoral fellowship from ICIQ International Postdoctoral Mobility Programme (ICIQ-IPMP), 2016.
- Humboldt Postdoctoral Fellowship, 2016 (not joined).
- JSPS Postdoctoral Fellowship, 2014.
- Selected for Poster Slam presentation, AsBIC 7, 2014.
- Honorable Mention Awards of IUPAC Prizes for Young Chemists, 2013.
- Junior and Senior Research Fellowship from CSIR, 2008–2012.

Research Interests

- Spectroscopic Characterization (X-ray crystallography, EPR, UV-Vis, NMR, UV-vis, resonance Raman, EXAFS) of high-valent 3d transition metal complexes and their proton coupled electron transfer reactivity studies.
- Understanding the effects of redox-inactive metal ions installed at the secondary Coordination Sphere on the Small Molecule Activation Reactions.
- Development of molecular electrocatalysts for different small molecule activation reactions.

IL-7

Leveraging Local Interactions to Affect Global Structures of Peptides and Peptidomimetics

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New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, Karnataka -560064, India
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Peptide-based drug design has attracted significant attention since the discovery of insulin for treating type II diabetes.[1] Today, more than 60 peptide-based drugs are available on the market, with over 140 in clinical trials.[1] However, the low bioavailability of peptides—due to their susceptibility to proteases and limited cell permeability—has shifted focus toward small molecule drug development.[2] While small molecules offer certain advantages, peptides possess unique potential for enhanced potency and selectivity, particularly in targeting large protein-protein interaction surfaces, which small molecules often struggle to engage effectively.[3] This has driven the development of "peptidomimetics"—peptide-like molecules engineered to retain the benefits of peptides, such as potency and specificity, while offering improved stability, protease resistance, and cell permeability.[4,5] Designing molecules that fold and function like peptides, while overcoming their inherent limitations, remains a challenging yet highly desirable goal. In this talk, I will explore the role of weak interactions in stabilizing well-defined peptidomimetic structures, with a particular focus on peptoids and azapeptides.[6,7] Additionally, I will discuss how these interactions contribute to the stabilization of polyproline II (PPII) and triple helical structures in collagen-mimetic peptides (CMPs).[8-10]

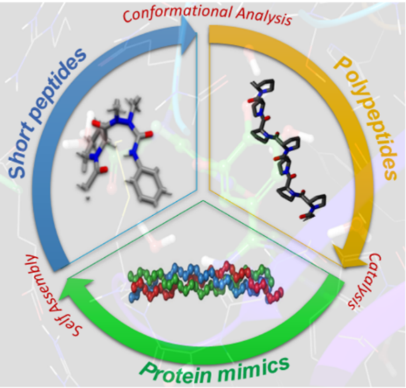

Figure 1. Peptidomimetic research at JNCASR.

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IL-7

Brief Biography

Bani Kanta Sarma

EDUCATION

8/2003 – 8/2008 PhD in chemistry, Indian Institute of Science, Bangalore, India (Best thesis award)

4/2001 – 4/2003 MSc. in Chemistry, Indian Institute of Technology, Guwahati, India. (1st rank)

POSTDOCTORAL EXPERIENCE

1/2009 – 5/2009 Postdoctoral Research Associate, UT Southwestern Medical Centre, USA.

6/2009 – 1/2014 Postdoctoral Research Associate, The Scripps Research Institute (TSRI) Florida, USA.

ACADEMIC CAREER

22/09/2023-present Associate Professor, New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore-560064

2019-2023 Faculty Fellow, New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research

03/03/2014-09/10/2019 Assistant Professor, Department of Chemistry, Shiv Nadar University, UP-201314

AWARDS/FELLOWSHIPS

2008 “Prof. S. Soundararajan Medal” the Best Thesis Award in Inorganic Chemistry for the academic year 2008-09.

2003 Silver Medal-First Position (CPA 9.59/10) in M.Sc. in Chemistry from IIT Guwahati

SELECTED PUBLICATIONS

1.Deka, J. K. R.; Sahariah, B; Sarma, B. K.* J. Org. Chem. 2023. https://doi.org/10.1021/acs.joc.2c01891.

2.Anshulata, Vishnoi, P.; Sarma, B. K.* Chem. Eur. J. 2023, 30, e2023033.

3.Deka, J. K. R.; Das, P.; Borah, D.; Vishnoi, P.; Sarma, B. K.* Chem. Commun. 2023, 59, 6080-6083.

4.Baruah, K.; Kalita, D.; Sahariah, B.; Deka, J. K. R.; Vishnoi, P.; Sarma, B. K.* Chem. Eur. J. 2023, 29, e2023001.

5.Sahariah, B; Sarma, B. K.* J. Phys. Chem. B. 2021,125, 49, 13394-13405.

6.Deka, J. K. R.; Kalita, D.; Sahariah, B; Sarma, B. K.* Chem. Commun. 2021, 57, 11236.

7.Kalpita Baruah, Sahariah, B; Sakpal, S. S.; Deka, J. K. R.; Bar A. K.; Bagchi, S.*; Sarma, B. K.* Org. Lett. 2021, 23, 13, 4949–4954.

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IL-8

Computational chemistry to understand light matter interaction

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Light matter interaction is central to life itself. It spans from prebiotic chemistry to vision, photosynthesis to skin photophysics. In this talk, I will discuss the computational techniques that can be used to understand these processes. The biological pigment melanin is the primary component in our skin that is responsible for photoprotection from sunlight. While this fact is well acknowledged, the exact molecular mechanism of the process is much more obscure. It is further complicated because of the lack of knowledge about the exact structure of melanin. We use computational tools to understand the mechanism of photoprotection in melanin [1,2] and find the crucial role of heterogeneity is central to efficient nonradiative decay without any structural damage.[3] To understand such processes we develop methods that are capable to deal with strongly correlated systems, such as density matrix renormalization group.[4-6]

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6. Bhattacharjee, I.; Ghosh, D.; Paul, A; *Chemical Science*, **2020**, *11*, 7009.

IL-8

Brief Biography

Debashree Ghosh

Prof. Debashree Ghosh obtained her M.S. degree in Chemical Sciences from IISc in 2005 and PhD degree from Cornell University, USA in 2010. She joined CSIR-NCL as a Senior Scientist in 2012, subsequently moving to Indian Association for the Cultivation of Science. Currently she is a professor at IACS. Her research focuses on the development of polarizable force fields and their hybrid frameworks with excited-state electronic structure methods, geared towards understanding the photo-physics of biological systems. She has been recognized by several awards, including the Annual Medal of the International Academy of Quantum Molecular Science (2021), SERB-POWER fellowship (2022) and Walter Kohn prize awarded by International Centre for Theoretical Physics (2022).

Research Interests:

1. Photo processes of biological systems
2. Development of methods for strongly correlated systems

Awards and Honours:

1. Emerging Investigator Lectureship award, PCCP (2018)
2. Annual Medal of the International Academy of Quantum Molecular Science (2021)
3. SERB POWER Fellowship (2022)
4. Walter Kohn prize by ICTP, Trieste (2022)
5. Editorial advisory board member of IJQC, Electronic Structure, Phys Chem Chem Phys, Mol. Phys., Journal of Chemical Sciences, J. Phys. Chem., J. Chem. Theory Comput., Chem. Soc. Rev.

IL-9

Modelling Intersystem Crossing in Metal-Free Organic Molecules for Efficient Triplet Photosensitization

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Department of Chemistry, Indian Institute of Technology Tirupati, Tirupati, A.P 517619, India
E-mail: **arun@iittp.ac.in**

Intersystem crossing is the key to realize the triplet photosensitization at the single molecular-scale. Large excited singlet-triplet gap and small spin-orbit coupling in heavy-metal free organic molecules limit the ISC and thereby, the triplet photosensitization efficiency. Molecular-twist and/or heteroatom substituents were shown to promote the ISC in several organic molecular systems.[1] Time-dependent density functional theory based computational modelling studies can provide a detailed understanding on the role of molecular-twist and/ or heteroatom substituents in tailoring ISC, which greatly helps designing efficient triplet photosensitizers. But, computational results, in particular excited-state energies and SOC are often highly dependent on the choice of density functional. Non-empirically and optimally tuned range-separated hybrid has been proven to produce a reliable and quantitatively accurate description of the excited-state electronic structures including SOC.[2,3]

In this talk, some of our recent computational findings on the triplet photosensitization in a few chalcogen-substituted π-conjugated organic molecules will be discussed. The excited-state electronic structures including the SOC are obtained from time-dependent optimally-tuned range-separated hybrid along with the ISC rates from Fermi-golden rule.[3-9] A reliable and predictive description of the ISC is thus achieved using quantitatively accurate energies of the electronically excited singlets and triplets combined with appropriate theoretical protocols. Importantly, molecular-level engineering of highly fluorescent organic molecules (such as perylenediimide and corrole) with chalcogen substituents is shown to yield high energy triplets required for photosensitization through efficient ISC due to the heavy-atom effect and also the excited-state symmetry differences.[4-9]

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4. R. Ahmed, A. K. Manna, *J. Chem. Phys.* **2022**, *157*, 214301.
5. R. Ahmed, A. K. Manna, *J. Chem. Phys.* **2023**, *158*, 214304.
6. P. Debnath, R. Ahmed, A. K. Manna, *J. Phys. Chem. B* **2023**, *127*, 10016.
7. A. M. Tedy, A. K. Manna, *J. Chem. Phys.* **2024**, *160*, 114306.
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9. A. M. Tedy, A. K. Manna, *Phys.Chem.Chem.Phys.* **2024**, DOI: 10.1039/D4CP03226H.

IL-9

Brief Biography

Arun K Manna

Educational and Professional Career:

Dr. Manna obtained his Ph.D. in Theoretical and Computational Chemistry from JNCASR, Govt. of India (2008-2012). Subsequently, he pursued his postdoctoral studies on electronic structures theories from Kent State University, USA (2012 to 2014) and from Weizmann Institute of Science, Israel (2015-2017). He started his independent career as an Assistant Professor in the Department of Chemistry, IIT Tirupati in 2017 and currently, holds an Associate Professor position.

Research Summary:

Dr. Manna research group at IIT Tirupati is engaged to study and explore the structure-property relationships of a range of functional molecules and extended materials at varied length scales by implementing modern state-of-the-art simulations methods rooted on electronic structure theory. Key properties of particular interests include optoelectronics, photovoltaics, energy-storage, photocatalysts, catalysis, transport, spintronic and thermoelectric for energy, health and environmental applications. Materials that are of prime focus include flexible organic, organic-inorganic hybrids and also low-dimensional systems. Reliable computational models and methods are implemented for achieving quantitative descriptions and also to provide robust predictions for new materials. As recent contributions, several metal-free organic molecules have been designed and proven to be efficient toward triplet photosensitization and improved photovoltaic performance. He has been authored of several articles published in internationally reputed scientific journals of high impact.

Honors and Awards:

- Teaching Excellence Award, IIT Tirupati (2024)
- DST Inspire Faculty Award, DST, Govt. of India (2017-2022)
- DST Early Carrier Research Award, SERB, Govt. of India (2018-2021)

IL-10

Enhanced Surface Processes of Carbonaceous Materials with Biocompatible Riboflavin

Arpan Kotal, Sawna Roy, Rajiv K. Kar*
Jyoti and Bhupat Mehta School of Health Sciences and Technology & Centre for Nanotechnology, Indian Institute of Technology Guwahati, Assam – 781039, India
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Carbonaceous materials including graphene oxide (GO and rGO), exhibit exceptional optical, thermal, and electrical properties, making them highly versatile for biomedical applications.[1] Their effectiveness in bioimaging, drug delivery, and sensing is linked to their tuneable surface chemistry, which heavily relies on dispersion stability [2]. This presentation will explore the significant role of riboflavin, a biocompatible molecule, in enhancing the surface properties and overall characteristics of GO/rGO nanosheet. Employing multidisciplinary techniques such as optical spectroscopy (UV-vis and fluorescence) we characterised the surface adsorption and electronic structure. Further, investigation of the dynamic insights into GO/rGO in complex with riboflavin was carried out using state-of-the art molecular computation. Additional characterization of the dispersed samples was conducted using X-ray diffraction, scanning and transmission electron microscopy, and Raman spectroscopy. Additionally, the cytocompatibility of these dispersed samples was investigated through *in-vitro* biological and antimicrobial assays, highlighting their potential for tailored biomedical applications [3].

We also conducted comparative analysis of the physico-mechanical properties of riboflavin-induced dispersed GO/rGO with both cationic surfactant (CTAB) and anionic surfactant (SDS) using tapping mode atomic force microscopy (AFM). Our investigation also encompassed charge distribution analysis and Young's modulus using amplitude modulation-frequency modulation AFM. These results demonstrate that riboflavin has potential to precisely tune material properties, making it a compelling biocompatible alternative for enhancing surface properties.

References

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IL-10

Brief Biography

Rajiv K. Kar

Dr. Rajiv K. Kar is an Assistant Professor at the School of Health Science & Technology, IIT-Guwahati. Previously, he worked as a Scientist in the Technische Universität Berlin, Germany. He did his PostDoc from The Hebrew University of Jerusalem, Israel & PhD from Bose Institute, India. Dr. Rajiv's research interest is in the field of medical device and diagnostics, biomaterials, and nanotechnology. His work include both experimental and theoretical methods.

Affiliation

Jyoti and Bhupat Mehta School of Health Sciences and Technology, &

Centre for Nanotechnology,

Indian Institute of Technology Guwahati, Assam, India

Experience

Since 2021: Assistant Professor at JBM School of Health Sciences and Technology, IIT Guwahati
Academic Editor: Plos One & Scientific Reports.

IL-11

Smart Biodegradable Microgels: A Versatile Platform for Diverse Applications

Garima Agrawal*
School of Chemical Sciences, Indian Institute of Technology Mandi, Kamand, Mandi-175075, Himachal Pradesh, India
(garima@iitmandi.ac.in)

Microgels are aqueous, three dimensionally crosslinked polymeric networks. Microgels belong to a special class of colloids that exhibit various attractive features including adjustable size and size distribution, chemical functionality, surface charge, and swelling degree.[1] Additionally, ease of post-modification, their large surface area for multivalent bio-conjugation, flexibility and softness, superior colloidal stability and stimuli responsive behaviour (sensitivity to T, pH, ionic strength) enable them as a versatile platform for diverse interdisciplinary applications.[1,2]

In keeping with the latest developments in multidisciplinary research, we have been trying to tap the potential of smart microgels for sustainable agriculture and cancer therapy **(Figure 1)**.[2,3] An overview of how multifunctional microgels, built on intuitively chosen molecular/macromolecular building blocks, could be exploited for controlled release under complex conditions as a way to develop smart sustainable carriers of fertilizers or drugs will be presented.[4,5] The capability of such microgels to perform multiple tasks, in terms of value addition even after their degradation, will also be discussed.[6]

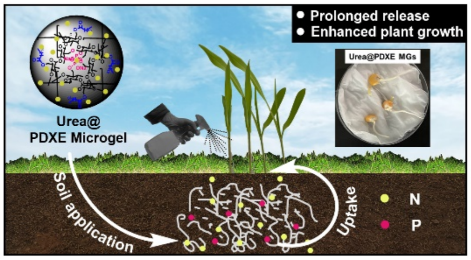

Figure 1. Environment friendly dextrin based microgels for sustainable agriculture.

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IL-11

Brief Biography

Garima Agrawal

Garima Agrawal did her M.Tech. in polymer science & technology at the Indian Institute of Technology Delhi, India. During her M.Tech., she received the DAAD Fellowship to carry out a research project at RWTH-Aachen University in Germany. After completing her Ph.D. at DWI Leibniz Institute for Interactive Materials - RWTH Aachen University, Germany in 2015, she joined postdoc at the University of Ghent, Belgium. In 2016, she was appointed as DST Inspire Faculty at Indian Institute of Technology Roorkee, India. Currently, she is working as an assistant professor at School of Chemical Sciences, Indian Institute of Technology Mandi, India. She is the recipient of several prestigious awards including NASI Platinum Jubilee Young Scientist Award 2022 from National Academy of Sciences India, DST Inspire Faculty Award 2016 from Government of India, and Young Achiever's Award 2023 from IIT Mandi. Her research interests include the synthesis of functional polymers based novel micro/nanomaterials and using them for designing interactive materials with active properties for targeted applications.

IL-12

Frustrated Lewis Pair-Like Activation of Small Molecules by An Azomethine Ylide with a Counter-Intuitive Bias for CS_2 over CO_2.

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Department of Chemical Sciences, IISER Kolkata, Mohanpur, West Bengal – 741246, India
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Azomethine ylides are typically transient synthons, heavily used in constructing N-heterocycles by dipolar cycloaddition reactions.[1] Presenting here a pyridyl-tethered isolable azomethine ylide (**AY**)[2] that unprecedentedly acts as a Frustrated Lewis Pair (FLP)[3] by activating various E–H (E = B, Si, O) bonds across its 1,3-dipolar carbons and a H–Al bond by its 1,5-dipole (C^+/N^-). It also cleaves a B–B bond but in an intriguingly different way, by oxidative addition at a carbene center formed in situ in the reaction through a 1,3-H^+ switch. Although a H_2 activation is unsuccessful, NH_3•BH_3 transfer hydrogenates **AY** readily. **AY** further undergoes cycloadditions with a few dipolarophiles, among which the addition of CS_2 but not CO_2 is alluring and counter-intuitive. DFT analyses well-justify the bond activation mechanisms in most of the cases and establishes a rationale for the CS_2 vs. CO_2 discretion.

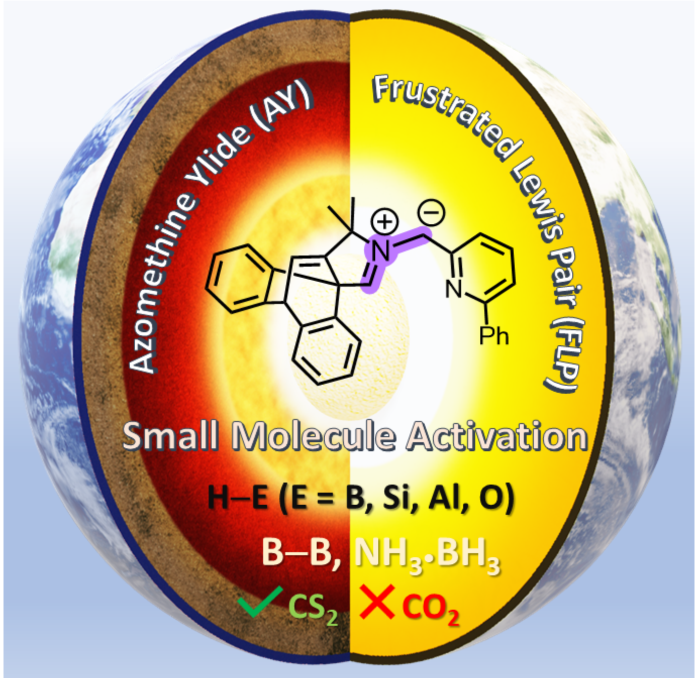

Figure 1. An isolable azomethine ylide unprecedentedly acting as a frustrated Lewis pair (FLP) in activating a series of small molecules including a counter-intuitive discretion between CS_2 and CO_2.

References

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IL-12

Brief Biography

Debabrata Mukherjee

Dr. Debabrata Mukherjee is an Assistant Professor in the Department of Chemical Sciences at the Indian Institute of Science Education and Research (IISER) Kolkata, located in Mohanpur, West Bengal. He holds a Ph.D. in Inorganic Chemistry from Iowa State University, USA, under the supervision of Prof. Aaron D. Sadow, following his M.Sc. in Inorganic Chemistry and B.Sc. in Chemistry (Hons.) from earlier academic pursuits. Dr. Mukherjee has been distinguished by significant academic recognitions, including the prestigious Alexander von Humboldt Postdoctoral Fellowship at RWTH Aachen University, Germany (2015-2017), where he worked under the guidance of Prof. Jun Okuda, and the Ramanujan Fellowship (2018-2023). His academic journey also includes research work at the Indian Institute of Technology Kanpur under Prof. V. Chandrasekhar.

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IL-13

Cyclizative Functionalization of Alkynols through Propargyl-Claisen Rearrangement

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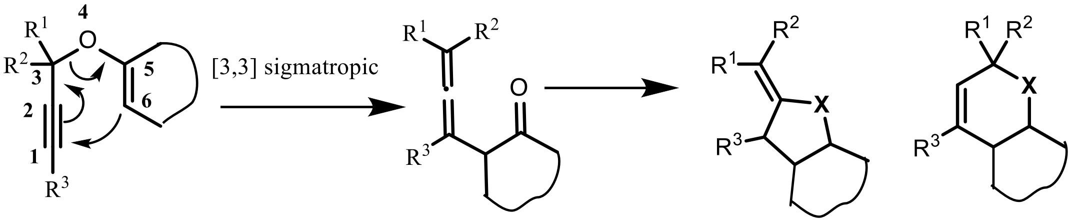
Claisen rearrangement[1] is one of the fundamental reactions of organic chemistry that is described as the [3,3]-sigmatropic transformation of allyl vinyl ether into γ, δ-unsaturated carbonyl compound. Many variations of this reaction are known regarding the substitution pattern of the vinyl group or the introduction of an aryl group, heteroatoms (most commonly Nitrogen or Sulphur) or a propargyl group. After fifty years of the first report by Claisen, it was in 1963 that the first successful attempts at the rearrangement of a propargyl aryl ether were reported.[2] Next, aliphatic propargylic Claisen rearrangement was reported in 1965.[3] Nowadays, Propargyl Claisen rearrangement is an excellent protocol for accessing many functionalized allenes through the [3,3]-sigmatropic transformation of propargyl vinyl ethers 3 (Scheme 1). Although allenes are excellent intermediates en route to other arrays of functional groups. Indeed, a wide range of important organic compound classes have been synthesised this way. More importantly, they are often synthesized without the need to isolate the allene intermediates, via domino reactions that always begin with the Claisen rearrangement.[4]



mono cyclic to polycyclic

Calcium(II)-Catalyzed, Highly General and D O M I N O reactions

Figure 1. Schematic representation of Propargyl-Claisen Rearrangement

We have developed a one-pot domino/sequential cyclization reaction to construct a variety of important privileged molecules through Propargyl-Claisen rearrangement commencing from readily preparable propargyl alcohols and ambident enols using sustainable Ca(II) based Lewis acid catalysts.[5]

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IL-13

Brief Biography

Srinivasarao Yaragorla

Srinivasarao Yaragorla graduated with M.Sc. degree in School of Chemistry from University of Hyderabad and obtained Ph.D. in synthetic organic chemistry from Indian Institute of Chemical Technology, Hyderabad in 2008. He subsequently held postdoctoral positions at the University of Minnesota and the University of Hyderabad as a DS Kothari Fellow. He worked as an Assistant Professor at the Central University of Rajasthan before joining the University of Hyderabad. Presently, he is a full professor at the School of Chemistry, University of Hyderabad.

His group works on various aspects of synthetic organic chemistry, including cyclizative functionalization of alkynols, Propargyl-Claisen rearrangement, C-H functionalizations, Donor-Acceptor cyclopropanes, Multicomponent cyclizations of a-Imino ketones and Mechanochemistry.

He is a recipient of the Chancellor Award and Associate Fellow of the Indian Academy of Sciences and the Telangana Academy of Sciences. Besides, he is a recipient of the International Travel Grant and Fast Track Young Scientist Awards from DST. He is a reviewer for many national and internationally reputed journals.

Prof. Srinivasarao Yaragorla published more than 80 research papers in national and internationally reputed journals and authored two book chapters. He has guided 8-PhD students and 7 PDFs. Prof. Yaragorla delivered more than 50 lectures at both national and international conferences.

IL-14

Design and Utilization of Metal Catalysts for Selective C-C and C-O Bond Forming Reactions

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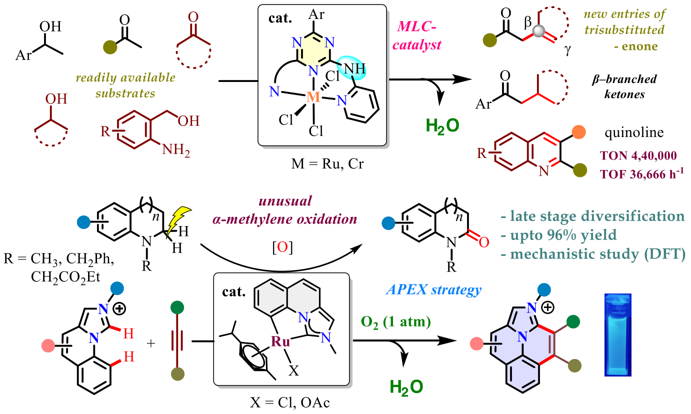
Abstract:

Metal-complexes are convenient tools in bond-forming reactions in organic synthesis. Their long-term stability and easy functionalization have allowed the development of novel catalytic systems that have had a tremendous impact in various areas of chemistry. The current paradigm primarily focuses on a single active metal site along with the ligands that impart electronic tunability to achieve the substrate binding and activation. In addition, metal-ligand cooperative (MLC) strategy is another important tool to activate the small molecule effectively. Nevertheless, less attention has been made to the molecular level understanding of electron-poor metal complexes in catalysis, particularly MLC pincer complexes with electron-poor ligand system in catalysis. Owing the motivation of unique electronic feature, herein the present work will be discussed on exploring the electron-poor MLC pincer complexes in synthetically challenging catalytic cross-coupling reactions of ketones and bio-renewable alcohols:[1] The electron-deficient triazine-core bearing NNN-pincer ruthenium(III) and cost-effective chromium(III) complexes are employed in this study towards sustainable synthesis of β-branched ketones and bio-relevant *N*-heteroaroamtic compounds like quinoline, qunazoline derivatives. By simply replacing the pyridine core to the central triazine-ring corresponding pincer complexes showed unprecedented catalytic activity and long life time in some cases, reaching TONs in the millions. Furthermore, rigid π-conjugated fused imidazo[1,5-*a*]quinoline (ImQ)-based cyclometalated ruthenium (II)[2] catalysed unusual α-methylene oxidation of synthetically diverse *N*-substituted tetrahydroquinoline to lactams and aerobic oxidative annulation reaction of alkynes will be discussed. In all case detail mechanistic insight will be disclosed with the help of kinetic studies, and DFT calculation.



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IL-14

Brief Biography

Animesh Das

Dr. Animesh Das was born in Midnapur, West Bengal, India. He obtained his B.Sc. degree majored in Chemistry at The University of Calcutta in 2004 and M.Sc. degree in Chemistry in 2006 at the Indian Institute of Technology, Kanpur, U.P, India. He then pursued his doctoral studies with Prof. Dr. Franc Meyer at the University of Goettingen, Germany. Later on he moved to University of Frankfurt in Germany, and University of Texas at Arlington, Texas, USA for his post-doctoral studies with Prof. Dr. Matthias Wagner and Prof. H. V. Rasika Dias, respectively. Dr. Das embarked on his independent career as an Assistant Professor, The Department of Chemistry, Indian Institute of Technology Guwahati in 2015. In 2021, he has been promoted to the rank of Associate Professor in Chemistry.

- His research interest is organometallic chemistry and catalysis, C-H activation and functionalization of small molecules for fuels and fine chemicals.

- Number of publications: 40.

IL-15

Simulating Multi-substrate bound state of Cytochrome P450

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Cytochrome P450cam (CYP101A1) is one of the most extensively studied metalloenzymes, known for catalyzing the native substrate camphor through binding at its core heme active site. Previous investigations[1], including one of ours, have consistently supported this understanding. However, as would be described in this seminar, to our surprise, we recently observed spontaneous formation of three-substrate bound state, during unbiased molecular dynamics simulations[2]. This observation is robust at both higher and lower substrate concentrations. This multi-substrate bound state, referred hereby as the "*3site State*," involves P450cam simultaneously binding to three substrate molecules at three distinct locations around the protein: the well-established "catalytic" site, the recently reported "allosteric" site, and an additional "waiting" site along channel leading to active site. The validity of this multi-substrate bound state has been further confirmed by in-vitro Nuclear Magnetic Resonance (NMR) measurements, suggesting that this might be the solution state of substrate-bound P450cam.

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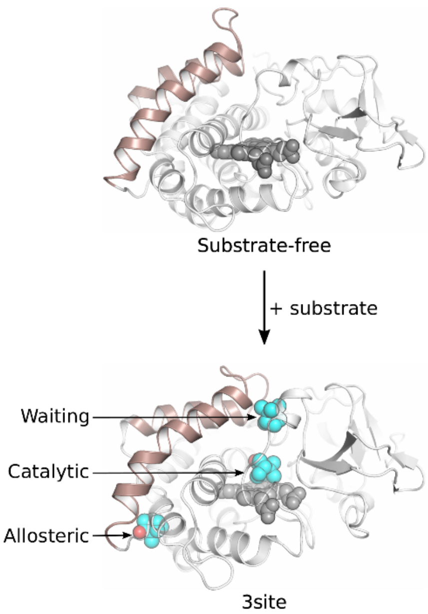

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IL-15

Brief Biography

Jagannath Mondal

Dr. Jagannath Mondal, born on March 17, 1983, is currently an Associate Professor at the Tata Institute of Fundamental Research, Hyderabad (TIFR-H). With a distinguished career in theoretical and computational chemistry, Dr. Mondal has contributed extensively to understanding chemically and biologically relevant processes. He holds a strong academic foundation, securing the first rank in B.Sc. Chemistry at the University of Calcutta in 2004 and earning the prestigious Hirschfelder Fellowship during his graduate studies at the University of Wisconsin-Madison in 2006. After completing his Ph.D., he undertook postdoctoral research with Bruce J. Berne at Columbia University, New York, from 2011 to 2015.

Dr. Mondal joined TIFR-H in 2015 as a Reader and was promoted to Associate Professor in 2021. His research focuses on computer simulations of biomolecular recognition processes, protein folding, osmolyte interactions, and the modeling of biological membranes and their protein interactions. He also explores integrative modeling of bacterial and eukaryotic cytoplasmic organization, electrocatalytic reactions, and transport across supramolecular assemblies.

Recognized for his contributions to science, Dr. Mondal has received numerous accolades, including the Alexander von Humboldt Fellowship for Experienced Researchers (2024–2026), the CRSI Bronze Medal (2024), and the TIFR-Infosys Leading Edge Grant Award (2022). He has been inducted as an Editorial Advisory Board Member of the Journal of Physical Chemistry (2024–2027) and was an Associate of the Indian Academy of Sciences (2016–2019). His earlier achievements include the Ramanujan Fellowship (2015–2020) and the Hirschfelder Fellowship. Dr. Mondal's expertise spans biomolecular simulations, drug discovery, and materials science, making him a leader in the field.

Dr. Mondal can be reached at his TIFR-H address in Hyderabad or via email at jmondal@tifrh.res.in or Jagannath.mondal@gmail.com. More details about his work are available on his webpage.

IL-16

Light-Camera-Action: Shining Visible Light on Hantzsch Ester

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Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar, Punjab – 140001, India
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When exposed to light, molecules in an electronically excited state undergo fascinating chemical reactions distinct from their behavior in the ground state.[1] This captivating principle lies at the core of photochemistry, giving rise to unprecedented transformations. In excited state, a molecule can serve as a superior electron donor (reductant) or a more effective electron acceptor (oxidant), capabilities unattainable through conventional ground-state reactivity.[2]

The redox reaction found in almost all living cells involves the conversion between NAD+ and NADH. This process is essentially a hydride (H^-) transfer reaction. In the realm of synthetic organic chemistry, the structurally similar 1,4-dihydropyridine (1,4-DHP) or Hantzsch ester has emerged as a promising hydride source in its ground state, commonly used in catalytic hydrogenation reactions.[3] Recent research has unveiled its potential to act as a strong photoreductant or as a source of hydrogen atoms via a single electron transfer (SET) process when exposed to visible light.[4]

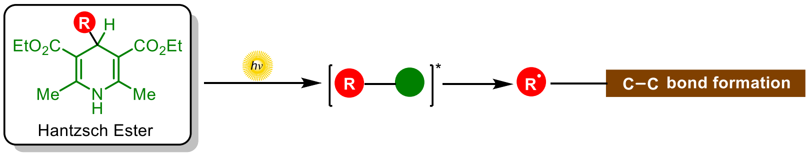

Figure 1. Graphical abstract of the generation of radicals from Hantzsch Ester

Moreover, structurally resemble, 4-alkyl-1,4-DHPs, in its excited state can act as a source of alkyl radicals without the need for any photocatalyst, and the resulting radicals can be further utilized to form C-C bonds. Inspired by the groundbreaking work of Melchiorre, Nishibayashi, and others,[5, 6] our group has also demonstrated C(sp3)-C(sp3) cross-coupling using these 4-alkyl-1,4-DHPs.[7] The focus of this talk will primarily center on the potential of these DHPs to reduce challenging molecules or to leverage the generated alkyl radicals to create diverse molecular complexity.

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IL-16

Brief Biography

Indranil Chatterjee

Dr. Indranil Chatterjee obtained his B.Sc. from Calcutta University, India in 2006, and then he moved to IIT Kharagpur for his M.Sc. study. In 2008 he moved to Germany for his Ph.D. study at Westfälische Wilhelms-University Muenster under the guidance of Prof. Dr. Armido Studer, where his studies centred on catalytic asymmetric cycloaddition reactions. After finishing his Ph.D. study in November 2011, he joined as a Postdoctoral fellow with Prof. Paolo Melchiorre in ICIQ, Tarragona, Spain in March 2012. His area of research mainly focused on new organocatalytic cascade reactions. After that from 2014 to 2016 he did another Post-Doc with Prof. Martin Oestreich at the Technische Universität Berlin, concentrating his research on Lewis acid catalysis. In 2016 December he joined IIT Ropar as an Assistant Professor. Since August 2024 he is holding a position of Associate Professor at IIT Ropar, India.

Details of any fellowship/awards/honors

(i) National Scholarship in Secondary and Higher Secondary exam. (2000 & 2002).
(ii) Ph.D. scholarship of the International Graduate School of Chemistry (GSC-MS), University of Muenster, Germany (2008-2011)
(iii) Postdoctoral Fellowship at ICIQ, Tarragona, Spain (2012-2014)
(iv) Cluster of Excellence UniCat Fellowship for Postdoctoral Research at Technical University Berlin, Germany (2014-2016)
(v) Institute Best Teaching Award (2020).
(vi) Thieme Chemistry Journal Award, 2022.

IL-17

Harvesting Light for Developing Enantio-/Diastereo-/Chemoselective Transformations

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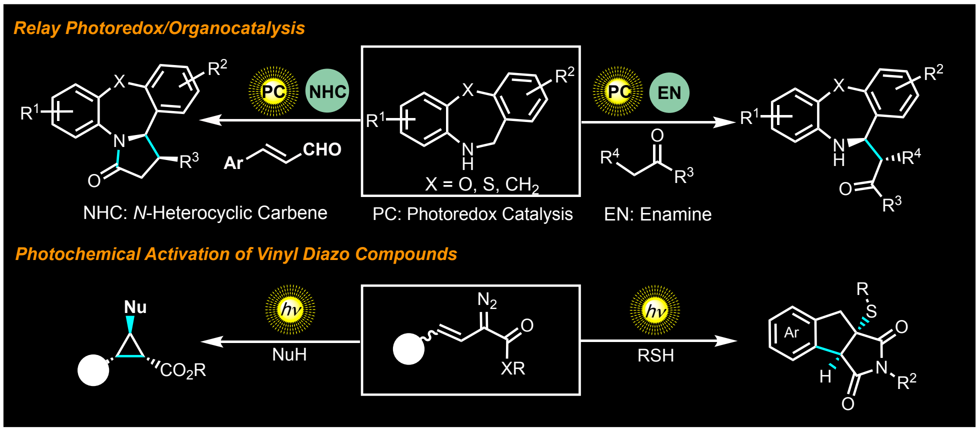
Applications of light energy to carry out organic reactions lead to orthogonal reactivities to that of ground-state thermal reactions. Previously, strong UV-radiations have been exploited to activate molecules, enabling them to react in the excited state. However, certain limitations are associated with these high-energy UV-light-driven organic processes, *viz.,* the requirement of specialized reaction vessels, undesired side reactions, and decomposition of reactants, thereby restricting its broad applications. Recently, the development of reactions under low-energy UV light and visible light, directly or facilitated with photocatalysis has opened new gates for efficient organic synthesis. The renaissance of photocatalysts led to tremendous progress in organic photochemical reactions by activating non-absorbing organic molecules with photo-redox catalysts. These developments provided new avenues for unusual reactivities and assessing complex molecular architectures with high selectivity, which have not been achievable through conventional organic synthesis. We have explored the applications of photoredox catalysis and direct activation of organic molecules with low-energy light to generate valuable reactive intermediates that have been probed further to discover new reactivities in highly chemo- and stereo-selective fashions. In this context, we have investigated the relay photoredox/organocatalysis for diastereo-/enantioselective synthesis of valuable seven-membered scaffolds.[1,2] Alternatively, we have developed photochemical chemo- and stereo-selective transformations of vinyl diazo carbonyl compounds.[3,4] The detailed results of our investigations will be presented.



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IL-17

Brief Biography

Pankaj Chauhan

Education:

- **Ph.D.**, Guru Nanak Dev University, India (Ph. D. Supervisor - Prof. Swapandeep Singh Chimni, Ph.D. date: 29th November 2012). Thesis Title - **Enantioselective Carbon-Carbon Bond Formation Catalyzed by Cinchona-Derived Organocatalysts**.
- **M.Sc. Chemistry**, Guru Nanak Dev University, India (2007).
- **B.Sc.**, Himachal Pradesh University, India (2004).

Research Interests:

Asymmetric Synthesis, Organocatalysis, Photochemical and Electrochemical Organic Synthesis, Synergistic Catalysis, Domino/Cascade Reactions.

Awards and Honors:

1. **INSA Young Associate** (2024)
2. **RSC Research Fund** (2022)
3. **Thieme Journal Award** (2018)
4. **DST INSPIRE Faculty Award** (2016, declined).
5. **Postdoctoral Fellowship** from European Research Council (ERC).
6. Selected for "**Research in Paris**" France (2013, declined).
7. Selected for "**Science without Border**" Brazil (2013, declined).
8. **International Travel Grant** by DST India (2011).

Positions Held:

1. **Associate Professor** at IIT Jammu (August 2023-till date)
2. **Assistant Professor** at IIT Jammu (October 2017-August 2023)
3. **Sub-Group Leader** with Prof. Dieter Enders at RWTH Aachen University, Germany (April 2014-September 2017).
4. **Postdoctoral Researcher** with Prof. Dieter Enders at RWTH Aachen University, Germany (April 2013-March 2014).
5. **Research Associate** with Prof. Swapandeep Singh Chimni at Guru Nanak Dev University, Amritsar, India (November 2012-March 2013).

IL-18

Ligand-Centered Redox Induced Chemical Transformations

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Abstract: The chemistry of transition metal complexes of redox-noninnocent ligands has gained immense attention over the years because of its interesting electronic structures. Over the decades, the primary research in this area was focused on understanding the ambiguous electronic structure and bonding of such complexes. Only in the last decade, it has shifted more to catalysis and, very recently, towards more physical applications upon realizing the fact that redox-noninnocent ligands, other than coordinating metal ions and offering steric control, can participate synergistically with the metal ions during electron transfer events and influence a chemical transformation in many ways.

This lecture will focus on various ligand-centered redox-induced chemical transformations, both stoichiometric and catalytic. A few examples will be discussed, including how interconversion between mono- and multi-metallic complexes can be achieved by controlling the ligand-centered redox events. Particular emphasis will be given to how radical-type reactions can be achieved in a controlled manner using 3d-metal-catalysts, avoiding thermodynamically unfavorable metal-centered redox events and making the overall process more eco-friendly and sustainable.

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IL-18

Brief Biography

Nanda Dulal Paul

Dr. Nanda Dulal Paul, originally from Kamakhyaguri, after completing his schooling from Kamakhyaguri High School, passed B. Sc, with Chemistry (Hons.) from St. Xaviers College, Kolkata in 2005 and completed his M.Sc. in chemistry with Inorganic Chemistry specialization in 2007 from the University of Calcutta. He did his Ph.D. at the Department of Inorganic Chemistry, IACS, Kolkata under the supervision of Professor Sreebrata Goswami from 2007-2012. In July 2012 he moved to the van't Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands as an ERC funded scientific researcher. Before completing his tenure as a Scientific Researcher at HIMS with Prof. Bas de Bruin, he was offered the position of Assistant Professor at the Department of Chemistry, IIEST, Shibpur in January 2014. Presently he holds the position of Associate Professor at the Department of Chemistry. He is married to Sutanuva and has two little sons Navayan and Suvayan.

Academic Qualifications

Scientific Researcher, Van't Hoff Institute of Molecular Science, University of Amsterdam, Amsterdam, The Netherlands, 2012-Dec 2013. (With Professor Bas de Bruin)
Ph. D. in Science, IACS (Jadavpur University), Kolkata, India, 2012 (Advisor: Professor Sreebrata Goswami)
M. Sc. University of Calcutta, 2007
B. Sc., St. Xavier's College, Calcutta University, 2005

Research Statement

Synthesis of new ligands and catalysts, Homogeneous and Bio-inspired catalysis, Spectroscopy, X-ray crystallography, DFT, New redox non-innocent ligand design, Synthesis of new catalysts featuring cheap and earth abundant transition metal ions, Development of alternative approaches in homogeneous catalysis using ligand centered redox events, Metal catalyzed C-H functionalization/activation, Dehydrogenation and cross dehydrogenative coupling, Photo catalytic reactions.

Awards

- Thieme Chemistry Journals Award – 2024
- 2023 Professor D.K. Banerjee Memorial Lecture Award (by Department of Organic Chemistry, IISc, Bangalore)
- Young Faculty Research Award (by Alumni Association Washibgton Metro Area, and GAABESU Shibpur Foundation, USA)
- ERC fellowship for post-doctoral research at the Van't Hoff Institute of Molecular Sciences, University of Amsterdam, The Netherlands

IL-19

Developing sustainable luminescent nanomaterials for solar to chemical energy conversions through complete metal free approach

Santanu Bhattacharyya

Department of Chemical Sciences, IISER Berhampur

email address: santanub@iiserbpr.ac.in

Considering two major alarming problems of modern society, *i.e.*- a) global warming and b) gradual depletion of traditional fossil fuels, it is utmost necessary to shift towards the alternative energy resources. In this regard, photocatalytic H_2 evolution from water is considered one of the cleanest approach till date. H_2 is the cleanest fuel and does not produce any greenhouse gas upon direct combustion, or even while acting as a chemical feedstock for other transportable fuel generation. Therefore, it is highly desirable to produce efficient photocatalysts. Till date several advancements have been made with metal-based inorganic semiconductors. However, their practical applicability is still under debate considering the environmental sustainability, stability and economical expenses. As a result, it is essential to develop alternate photocatalysts that are environmentally sustainable, cost-effective, stable and highly efficient. The metal-free approach is one of the most promising approaches in contrast to the traditional metal based photocatalysts. In this regard, our major focus is to develop and optimize complete metal free sustainable nanomaterials made of earth abundant elements (*i.e.*- C, S, P *etc.*) for solar H_2 production and simultaneous chemical energy conversions through optimizing light-matter interactions and the desired photochemical processes for photocatalysis ranging from *ms* to *fs* time domain.

Reference: *a) ACS Appl. Mater. Interfaces 2024, 16, 28, 36763–36773*
b) J. Mater. Chem. A 2024, DOI:10.1039/d3ta07895g
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e) Adv. Opt. Mater. 2022, 10, 2102641
f) J. Phys. Chem. C 2024, 128, 37, 15286–15297

IL-19

Brief Biography

Santanu Bhattacharyya

Dr. Santanu Bhattacharyya is an Associate Professor in the Department of Chemical Sciences at Indian Institutes of Science Education and Research (IISER) Berhampur, specializing in Materials Science, Physical Chemistry, and Nanoscience and nanotechnology. Born on January 25, 1985, he is based at the Transit Campus in Ganjam District, Odisha. His research focuses on four key areas: developing sustainable semiconducting nanomaterials for photocatalytic conversions of solar energy into solar fuels and green chemicals, creating room temperature phosphorescent/afterglow materials for sensing and security applications, investigating fundamental light-matter interactions in light harvesting nanomaterials through ultrafast time resolved spectroscopy, and photo reformation of waste materials into value-added chemicals and waste water remediation. His work can be found on his personal homepage (https://sbch2008.wixsite.com/santanu) and Google Scholar profile, which showcases his contributions to sustainable energy and materials science research.

IL-20

Enhancement of Complexation due to the Bath Effect: A van der Waal Complex in N_2 Bath

M. S. Yadav,[a] S. S. Ahamed,[a,b], H. Mahanta,[a,c], A. K. Paul,*[d]

[a]*Department of Chemical and Biological Sciences, NIT Meghalaya, Meghalaya*
[b]*Department of Chemical Sciences, S. N. Bose National Centre for Basic Sciences, Kolkata*
[c]*Department of Chemistry, Kaziranga University, Assam*
[d]*Department of Chemial Sciences, Bose Institute, Kolkata*
e-mail: amit.paul@jcbose.ac.in

In this lecture, I shall be showing interesting results on the association and ensuing dissociation dynamics of the weakly-bound aromatic complexes if those take place in a bath of 1000 N_2 molecules. Benzene (Bz)-hexafluorobenzene (HFB) complex is taken for the study and the temperature range is considered as 1000-2000 K. N_2 bath densities of 20 and 324 kg/m^3 are taken. It is observed that with the increasing bath density, the association probabilities of the aromatic molecules increase with a decrease in dissociation rate.[1-3] Furthermore, the decisive role of the bath is explored in the dynamics of mode-selective excitation of Bz-HFB. During the dissociation dynamics, there is a huge competition between the dissociation and energy transfer pathways. In general, it is observed that higher the density of bath, higher will be the rate of energy transfer, higher is the association and lower is the dissociation. Thus, the complexation is increased for van der Waal complexes due to the energy transfer effect of the bath.

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2. S. S. Ahamed, H. Mahanta, and A. K. Paul, *Chem. Phys. Letts.* **2019**, *730*, 630-633.
3. S. S. Ahamed, H. Mahanta, and A. K. Paul, *J. Phys. Chem. J. Phys. Chem. A* **2019**, *123*, 10663 - 10675

IL-20

Brief Biography

Amit Kumar Paul

Dr. Amit Kumar Paul received his Bachelor's, Master's, and Ph.D. degrees from the University of Calcutta. He did his postdoc with Professor William L. Hase at Texas Tech University from 2013 to 2016.

He joined NIT Meghalaya in the middle of 2016 and served there for eight (08) years. Recently, he has moved to the Bose Institute, Kolkata as an associate professor.

Dr. Paul's research interests are in computational reaction dynamics in gas and condensed phases. He is currently involved in machine learning-based implementations of chemical dynamics problems. He also collaborates with more than five (05) experimental groups in India and abroad.

So far, he has published around sixty (60) papers in various national and international journals, has guided four (04) Ph.D. students for their degrees, and has secured multiple external research funding from SERB, CSIR, etc.

He was recognized with an excellent research Contribution award for the period 2022-23 by NIT Meghalaya. He is also serving as an editorial board member of the International Journal of Chemical Kinetics.

IL-21

Probing surface-ligand interactions in SCN^--capped quantum dots using 2D IR spectroscopy

Samadhan Deshmukh[a,b], Srijan Chatterjee[a,b], Sayan Bagchi[a,b,*]
[a] *Physical and Materials Chemistry Division, National Chemical Laboratory (CSIR-NCL), Dr. Homi Bhabha Road, Pune 411008, India*
[b] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India*
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The nanocrystal surface serves as a crucial interface bridging the semiconductor lattice and the encapsulating ligands, thereby exerting a substantial influence on the photophysical characteristics of semiconductor nanocrystals across a spectrum of applications. Enhancing the conductivity and carrier mobility of nanocrystal-based devices is attainable by substituting protracted organic ligands with concise inorganic counterparts. However, a comprehensive knowledge of the interplay between the inorganic ligands and the nanocrystals remains elusive, primarily due to the dearth of experimental methodologies directly investigating the inorganic ligands. In my presentation, I will discuss the findings of 2D IR spectroscopic investigations, shedding light on how variations in the dynamics of inorganic ligands within a heterogeneous nanocrystal ensemble offer insights into the diversities of inorganic ligand–nanocrystal interactions. Through these results, discernible ligand dynamics time scales in nanocrystals capped with SCN– ligands emerge as effective identifiers of discrete ligand populations, thereby imparting a molecular perspective into the intricacies of the nanocrystal surface. Furthermore, I will explore the modifications in the electrical double layer's presence in correlation with nanocrystal size variations. In summary, my presentation will elucidate the of 2D IR spectroscopy to unravel these dynamics to unlock a more comprehensive understanding of these interactions, thereby paving the way for novel applications and improved device performance.

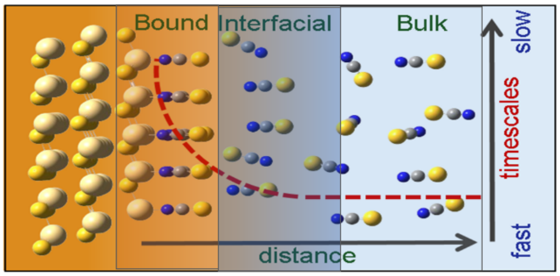

Figure 1. Graphical abstract of the surface ligand interactions between CdSe nanocrystals and SCN^- ions

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IL-21

Brief Biography

Sayan Bagchi

Dr. Sayan Bagchi holds the position of Senior Principal Scientist in the Physical and Materials Chemistry Division at CSIR-NCL, Pune. He earned his Ph.D. degree from the University of Pennsylvania (USA) in 2008. Following the completion of his Ph.D., Dr. Bagchi embarked on a post-doctoral research journey at Stanford University. In 2012, Dr. Bagchi joined NCL as a Senior Scientist.

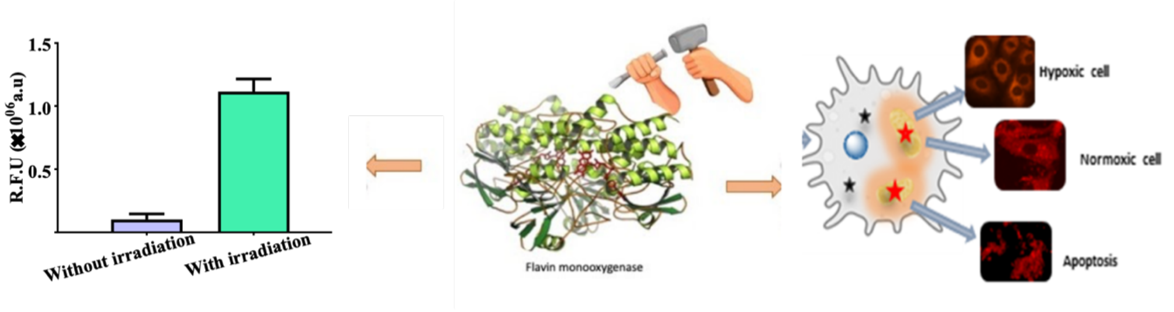
Bagchi research group conducts ultrafast two-dimensional IR experiments employing femtosecond pulses to capture spectral movies that illustrate molecular fluctuations. Dr. Bagchi's research interests encompass gaining spectroscopic insights into heterogeneous systems spanning the fields of chemistry, biology, and materials science. His approach involves a combination of experimental work and computational simulations to achieve a comprehensive molecular understanding of various chemical processes.

IL-22

Harnessing the photophysical nature of Flavin for biological applications

Ashutosh Kumar Mishra*
Indian Institute of Technology-Hyderabad-India
(Email: akm@chy.iith.ac.in)

Bioinspiration remains the most sought out platform for identification and exploration of the novel chemical construct for the desired application. For instance, the ubiquitous nature of the flavoprotein has attracted researchers since its discovery due to its involvement in range of enzymatic transformations playing a significant rile on numerous biochemical phenomena's.[1] Extensive efforts have been put together not only to understand its biological involvement but also to design and develop catalytic design based on the flavin core structure. Interestingly, while the catalytic capabilities of the flavin based system have been comprehensively explored; comparatively much lesser effort has been put together design synthetic analogue to harness the admirable luminescent nature of the flavin core.[2] While natural entity utilizes the intricate inter-play of the noncovalent interactions involving the apoprotein matrix to fine tuning of the functional behavior for desired purpose. Judicially design synthetic analogue might offer a simple and robust chemical model with similar functional capabilities. Our group at IIT-Hyderabad, is working on the design and development of the flavin based synthetic constructs for diverse applications.[3] Herein this talk, I will be discussing in the design and development of the flavin based models as a potential chemical construct for biomedical applications.[4]



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IL-22

Brief Biography

Ashutosh Kumar Mishra

Ashutosh Kumar Mishra obtained his master's degree in chemistry from DDU Gorakhpur university and moved to Indian institute of technology-Kanpur to work on scalable structural complexities in metal-nucleobase interactions. His doctoral thesis fetch him Eli Lilly outstanding thesis award-First prize in 2011. Later he moved to Northwestern University (USA) as post-doctoral fellow to work on understanding the underlying mechanism and dynamic of charge transport phenomenon in synthetic model DNA systems. Moving back to India as assistant professor at Indian Institute of technology-Hyderabad, where he is currently serving as associate professor. His research group is interested in bioinspired model systems with subtle modification around the flavin core chemical skeleton to fine tune the functional behaviour for potential application in catalytic, bioimaging or generating higher order architecture.

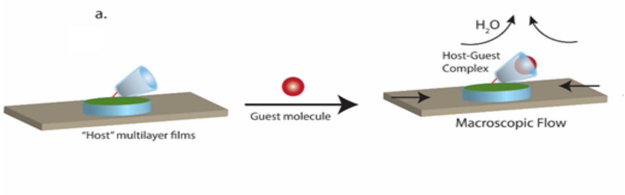
IL-23

Autonomous fluidics: A chemically powered self-sustained motion.

Debabrata Patra*

Institute of Nano Science and Technology, SAS Nagar, Punjab, 140306, India
(patra@inst.ac.in)

Autonomous fluidic systems that are capable of turning "on" in response to specific analytes and providing precise control over the flow rate without aid of any external power source offer considerable promises in next generation smart devices. Recently, autonomous motion that arises from the catalytic harnessing of chemical free energy from the surrounding environment has been demonstrated at the nano- and microscale. Tethering these catalytic systems to the surfaces enables the transfer of the mechanical force to the surrounding fluid. For example, surface-bound enzymes act as pumps in the presence of their specific substrates and driving large scale fluid flows.[1] Furthermore, the fluid velocity increases with increasing reaction rate which depends on concentration of the substrate. Despite the impressive progress, these micropumps are still fuel specific which limits their practical applications. An ideal pump should turn on autonomously by exposure to a chemical signal and thus would enable fluid flow that can be controlled by the presence and concentration of a specific analyte.



Scheme: "Host-Guest" recognition mediated fluid flow

In this context, the supramolecular approach mediated by "host-guest" interactions can play a pivotal role for designing of a micropump where wide range of "guest" molecules can act as a fuel for the systems. In the first approach, β-cyclodextrin "host" functionalized multilayer films were constructed via layer-by-layer assembly and the micropumps turned on fluid flow upon the addition of "guest" (1-adamantylamine and ferrocenecarboxylic acid) molecules to the films. The rise of convective flow is primarily due to the solutal buoyancy caused by "host-guest" molecular recognition.[2] In a different approach, the reversible and dynamic nature of supramolecular assembly was exploited to showcase valveless flow reversal in a pH responsive microsystem.[3] Moreover, these supramolecular interfaces could amplify weak molecular signals to visible output. The multilayer films were employed to discriminate chiral enantiomers and geometric isomers by fluid flow response.[4] Finally, we have deciphered the geometric self-sorting of pillar[n]arenes by analyzing flow patterns.[5] These types of microscale devices will be useful in diverse applications ranging from microanalysis and microfluidics to single-use diagnostic devices.

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IL-23

Brief Biography

Debabrata Patra

Dr. Debabrata Patra is a Professor and Head of the Energy and Environment Unit at the Institute of Nano Science and Technology (INST) in Mohali, Punjab, India, with a distinguished academic background including a Ph.D. in Chemistry from the University of Massachusetts, Amherst, under Prof. Vincent M. Rotello's supervision, and postdoctoral experiences at the University of Zurich, Texas A&M University, and Pennsylvania State University. His research spans critical areas of nanotechnology, including self-assembly and jamming of colloids, self-powered supramolecular assembly, enzyme-powered motion, supramolecular nanomotors, and macroscopic self-assembly. Currently serving as a Professor at INST since January 2023 (and previously as an Associate Professor from 2016-2022).

IL-24

Ferrocene functionalized bimetallic catalysts for water oxidation

Biswajit Saha*

Advanced Materials Group, Materials Sciences and Technology Division, CSIR-NEIST, Jorhat-785006, Assam

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Generation of green energy is a one of the major challenges in modern catalysis chemistry.[1] Plants directly store solar energy in the form of chemical energy during photosynthesis. Mimicking photosynthesis in the lab is inherently challenging because of infeasible thermodynamic and kinetic inertness.[2] In our lab, we have focused on the oxygen production from water.[3] For this purpose, we have attached a second metal in the form of ferrocene in well-established complexes and compared the catalytic activities of both. In every attempt, better yields of oxygen were obtained on attaching a ferrocene framework. A bimetallic synergy between the two metals was proposed to explain this increment. Identification of a few proposed intermediates spectroscopically of the mechanism have provided better insights.[4] DFT studies shed further insights to establish the role second metal. In this lecture key findings related to this synergistic effect will be discussed.

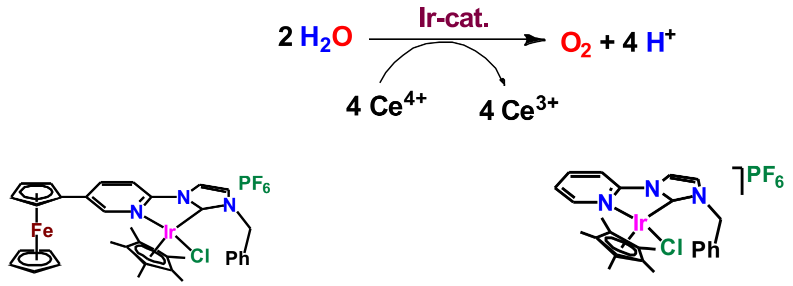

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Figure 1: Water oxidation with bimetallic catalyst

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IL-24

Brief Biography

Biswajit Saha

Dr Biswajit Saha has finished his BSc from Belur Ramakrishna Vidyamandiara under Calcutta University. He was the recipient Somnath Banerjee Memorial medal for securing 1st class in BSc. After qualifying JAM 2005 he completed MSc from IIT Kanpur. Then he has done his PhD with Prof Jitendra K. Bera from IIT Kanpur in the field of organometallic chemistry. He was awarded Eli Lily Best Thesis award with $1000 and a Plaque by NOST. He was Erasmus Mundus Post Doctoral fellow at Amsterdam University, The Netherlands with Prof. Vander Vlugt. He was PBC post doctoral fellow at Hebrew University, Israel with Prof Dmitry Gelman. In 2016 he has joined CSIR-NEIST as Scientist and in 2020 he is promoted to Senior Scientist. Two students have completed PhD under his supervision and two as co-supervisor. Presently two students are pursuing PhD with him. His research interest lies in the field of bimetallic catalysis where he focuses the synthesis of redox active ferrocene functionalized metal catalysts for small molecules activations. Till now he has finished two SERB funded projects and one CSIR-FBR project. Presently he is executing one CSIR project and one DRDO project at CSIR-NEIST, Jorhat.

IL-25

From Discovery to Fluorescence Thermometer via H- to J-Aggregate Switching: the Journey of Aldrone Condensation

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Department of Chemistry, Indian Institute of Technology Guwahati, Assam – 781039, India
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Abstract: Aldrone condensation is a reaction in which a C-nucleophile attacks to the N-atom of a nitro group, and produces **ald**onit**rone** after dehydration (Figure 1).[1] Although such nucleophilic addition to a nitro group was reported more than a century ago, albeit as a proposed intermediate during indigo synthesis by Baeyer,[2] the aldrone condensation remained elusive until last year. In many instances, other reactions were accompanied after nucleophilic addition to the N-atom. High reactivity or low stability of the product aldonitrone was thus a limiting factor for the successful completion of the aldrone condensation. Facile occurrence of other competing pathways, like single electron transfer or nucleophilic substitution of hydrogen atoms also diminished the probability of the aldonitrone formation.[3] On the top, surrounded by two bulky and electronegative O-atom, the electrophilic N-atom is not easily approachable by a nucleophile. In spite of the difficulties, we successfully accomplished the challenging reaction for the first time in 2023.[1] We have demonstrated the same using five different 5-alkylamino-8-nitro-1-acetylnaphthalenes, where intramolecular acid-catalyzed nucleophilic attack of enol moiety to the N-atom of nitro group produced α-keto aldonitrone, also known as *peri*-naphthoisatogen (PNTI), via addition-elimination mechanism. In similarities with aldol condensation, the reaction was named as aldrone condensation. The PNTIs showed characteristics of 1,3- dipole and reacted with ethyl acrylate to produce an isoxazolidine ring, which subsequently converted into aza phenalenone derivative via ring cleavage. Both the PNTI and the corresponding derivative are emissive, and absorb strongly in the visible region, displaying absorption maxima at 551 and 561 nm respectively. The PNTI showed interesting self-assembly behavior. In a THF-water mixture the dye produced non-emissive H-aggregate at room temperature, but converted in to emissive J-aggregate at elevated temperature.[4] The temperature-dependent emission behavior of the dye could be used as fluorescence thermometer. The journey of the aldrone condensation, from discovery to the application of the products, would be discussed in details.

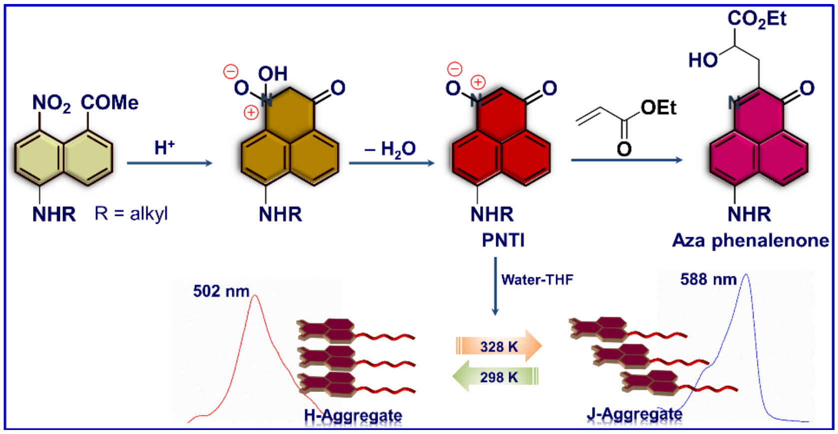

Figure 1. Acid catalyzed aldrone condensation, 1,3-diploar reaction of the of aldonitrone and its temperature dependent H- to J-aggregate switching.

References:

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IL-25

Brief Biography

Kingsuk Mahata

Kingsuk Mahata received his M.Sc. degree in chemistry from Indian Institute of Technology, Kanpur in 2005. Subsequently, he joined the research group of Prof. Schmittel at the University of Siegen, Germany, and obtained a Ph.D. on metallo-supramolecular chemistry in 2010. In the same year he moved to the University of Wuerzburg, Germany, and joined the research group of Prof. Frank Wuerthner as an Alexander von Humboldt fellow. In the beginning of 2013, he joined the chemistry department of Indian Institute of Technology, Guwahati as an assistant professor. From 2019, he has been working as an associate professor at the same institute. His research interests focus on synthesis, supramolecular polymerizations, and stimuli-controlled (metal, acid, light *etc.*) switching of *peri*-functionalized dyes. He is also actively pursuing the utilities of aldrone condensation, a newly invented reaction.

IL-26

Probing Aromaticity with Hydrogen Bonding in a Supersonic Molecular Jet

Himansu S. Biswal*
[1]*School of Chemical Sciences, National Institute of Science Education and Research (NISER), PO- Bhimpur-Padanpur, Via-Jatni, District- Khurda, PIN - 752050, Bhubaneswar, India*
[2]*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India*
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Aromaticity is a century-old concept that is even introduced in the high school textbooks. However, the determination of the order of aromaticity of as simple molecules as furan, thiophene and selenophene is still challenging. Different theoretical and experimental methods posit different aromaticity orders. For example, the most popularly used theoretical method, such as Nucleus-Independent Chemical Shift (NICS), predicts that selonophene is the least aromatic, whereas the ^{1}H NMR experiments suggest that selonophene is the most aromatic. We tested 21 aromaticity indices, but the conclusion varies from method to method. Hence, to benchmark the existing theoretical results and arrive at a concrete conclusion, mass-selective electronic and vibrational spectroscopy of these five-membered heterocycles in an isolated supersonic-jet-cooled condition was necessary. Since the aromaticity order can be unveiled from the magnitude of the electron density in the ring, we used hydrogen bonding as a probe. In this presentation, we wish to highlight the Supersonic jet spectroscopy facility built at NISER, which is used to study the structure and dynamics of molecules and molecular clusters that have been cooled to about 10-15 K (far below their boiling points) but remain in the gas phase. Cooling the internal degrees of freedom (molecular rotations and vibrations) through the isenthalpic expansion of the molecular jet with a speed higher than the speed of sound in a vacuum produces a highly resolved and simplified electronic and vibrational spectrum.

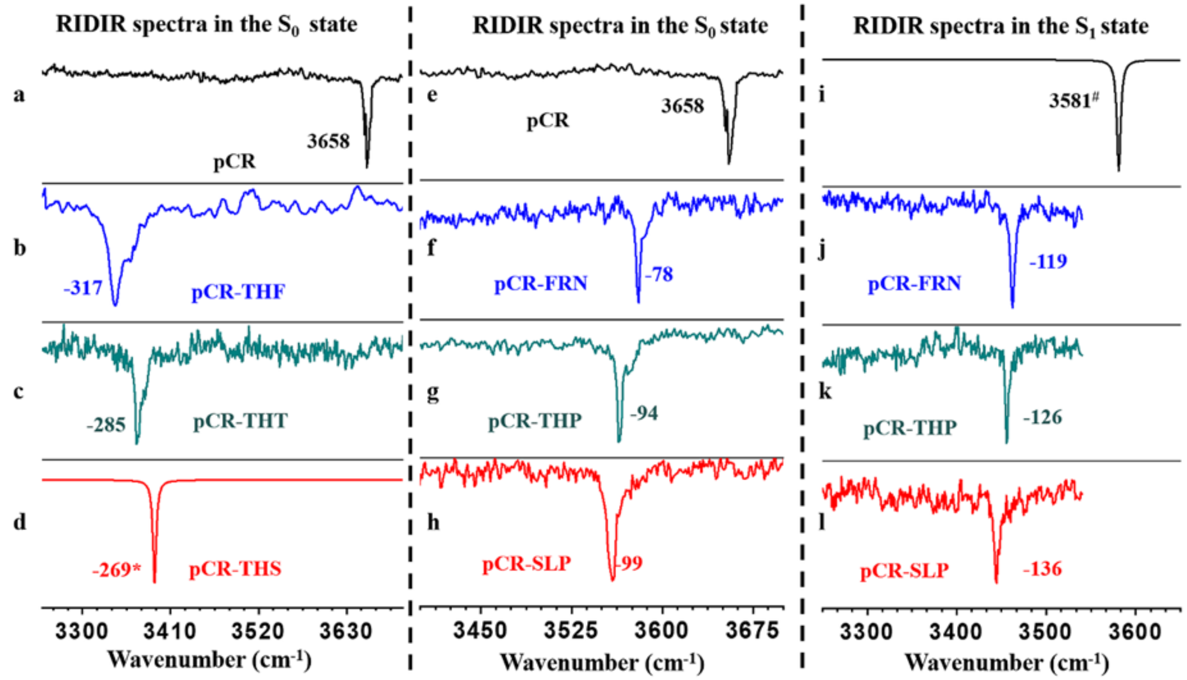

Figure 1. Mass selective IR spectroscopy to probe electron density and aromaticity in the five-membered heterocycles. Ground state (S_0-state) and first excited state (S_1-state) resonant ion-dip IR (RIDIR spectra of free para-cresol and its H-bonded complexes with the saturated and aromatic-heterocycles.

IL-26

Brief Biography

Himansu Sekhar Biswal

Ph.D. Institution, Year: Tata Institute of Fundamental Research (TIFR), 2009
Post Doctoral Research:
1. CEA, Saclay, France (2009-2011), PI: Prof. Michel Mons
2. University of Michigan, USA (2011-2012), PI: Prof. Jenifer Oglive

Affiliation: Professor at School of Chemical Sciences, NISER, Bhubaneswar; Homi Bhabha National Institute (HBNI), Mumbai (since July 2022)
Field of Research: Laser Spectroscopy, Chiroptical Spectroscopy, Instrumentation, and Computational Chemistry
Total Number of Publications/Patents/Books: 88 publications in high-impact journals (JACS, Angew. Chem., Chem. Sci., ACS Central Sci., JPCL, Acc. Chem. Res., Chem. Soc. Rev., Nat. Mat.)
Awards/Recognition Received:
1. Fellow of Royal Society of Chemistry (FRSC), UK (2023)
2. Featured in "Young Physical Chemists" - Journal of Physical Chemistry C (2019)
3. INSPIRE Faculty Fellow DST-INSA (2011)
4. Young Scientist Award, ISRAPS (2011)
5. Postdoctoral Research Fellowship, Dept. of Energy & University of Michigan (2011)
6. Best Thesis Award, TIFR (2009)
7. Multiple national scholarships from 1995-2003

Member of Learned Societies:
1. Royal Society of Chemistry (RSC), UK
2. Chemical Research Society of India (CRSI)
3. Indian Society for Radiation and Photochemical Sciences (ISRAPS)
4. National Magnetic Resonance Society of India (NMRS-India)
5. Indian Photobiology Society (IPS)
6. Indian Society of Atomic and Molecular Physics (ISAMP)
7. Orissa Chemical Society (OCS)
8. Association of Chemistry Teachers (ACT)
9. Indian Science Congress Association (ISCA)

IL-27

Nanofluidic Flow through Bio-Channels; a Novel Resource of Sustainable Energy

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Our group explores the confined space between the 2D layers for applications like harvesting electrical energy from nanofluidic ionic transport, ionic/molecular separation, and designing shape-morphing materials. While working on nanofluidic confinements, we were attracted towards bio- fibres enriched with nanoconfined fluidic channels. We are exploring the possibility of exploiting them for technological applications like nanofluidic energy harvesting or molecular separations. For example, we demonstrate that the biofluidic channels of coconut (or coir) fibres (CFs) can be an ideal platform for generating electricity from nanofluidic transport. During the flow of water, the channels of CFs generated electrical signals up to 35 mV and 42 nA. The power density obtained as such was drastically improved (up to 17-fold) upon modification of the delignified pores of CFs with two-dimensional flakes of graphene oxide (GO) and p phenylenediamine (pPDA). Modifying the coir channels also improved the breaking stress, and Young's CF by 671% and 3325%. Similarly, we also examined the possibility of utilizing bio- waste-derived electrolytes as an electrical energy resource by placing them across semipermeable membranes prepared through parallel stacking of coir fibres. The nanofluidic membrane (d-CF-V) prepared by modifying the inner walls of the bio-fluidic channels with atomically thin layers of vanadium pentoxide (VO) showed excellent perm-selectivity (t+= 0.876, with 1000-fold KCl concentration difference) and electricity conversion efficiency (~ 28.25 %). With simulated sea and river water, the d-CF-V yielded output energy up to 2.43 W/m2. The sun-dried Garcinia morella (Kuji thekera), and charred peels of Musa balbisiana (banana) were used here as sustainable sources of bio electrolytes, which in combination with permselective d-CF-V yielded a power density of about 1.4 W/m2, which was drastically improved by replacing standard Ag/AgCl electrodes with nanomaterials exhibiting contrasting charge transfer activities.

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IL-27

Brief Biography
Kalyan Raidongia

Dr. Kalyan Raidongia is an Associate Professor in the Department of Chemistry at the Indian Institute of Technology (IIT) Guwahati. His prolific career spans research in energy harvesting, smart materials, nanofluidic transport, self-healing materials, and water treatment technologies. With an impressive record of 63 publications in international journals, Dr. Raidongia's work has garnered over 4,372 citations, reflecting his significant contributions to the scientific community. He has also filed three patents, one of which has been approved, and successfully led 11 sponsored R&D projects, including eight government-funded and three industrial consultancy projects.

Dr. Raidongia's research group at IIT Guwahati comprises a dynamic team, with six Ph.D. students graduated, one thesis submitted, and eight ongoing Ph.D. projects. Additionally, he has supervised 20 postgraduate theses/projects. His academic background includes a Ph.D. in Chemistry (2011) and an M.S. in Materials Science (2008) under the mentorship of Prof. C.N.R. Rao and Prof. M. E Swaramoorthy at the Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore. He holds an M.Sc. in Chemistry (2005) from Gauhati University, Assam. He has held key administrative roles, including serving as Programme Officer for NSS-IIT Guwahati and as a member of DUPC, DPPC, TT Coordinator, and the Steering Committee for Institute Lecture Series. His professional journey includes a postdoctoral tenure (2011–2015) under Prof. Jiaxing Huang at Northwestern University, where he made groundbreaking advances in nanomaterials.

Dr. Raidongia has been recognized with prestigious honors, including being named an Emerging Investigator in Journal of Materials Chemistry A (2018), receiving the DST Ramanujan Fellowship (2015), and the International Institute for Nanotechnology Outstanding Research Award (2013). Among his notable recent publications are papers in high-impact journals such as Advanced Functional Materials, Nano Energy, and Nano Letters.

IL-28

Chemoselective Bioconjugation and Enantioselective Catalysis inside Protein Condensate

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Liquid-like protein condensates are ubiquitious in cellular system and are increasingly recognized for their roles in physiological processes.[1] Condensed phase harbors distinctive chemical microenvironment, markedly different than dilute aqueous phase. However, until now, chemoselective functionalization of proteins inside condensed phase and that too, under altering surrounding environment remains elusive. we demonstrate chemoselective modification pattern of nucleophilic canonical amino acid sidechains (namely – cysteine, tyrosine and lysine) of the protein towards 4-chloro-7-nitrobenzofurazan (NBD-Cl) in the dilute and condensed phase. Herein, how the effect of nucleotides and their enzymatic in situ dissociation temporally modulate the pH of the protein condensate and the corresponding chemoselective pattern of the protein will also be delineated.[2,3] We found the pH of the condensate decreases in the presence of nucleoside triphosphate, whereas it increases in the presence of nucleoside monophosphates or free phosphate ion (Pi). For instance, lysine-specific modification gets inhibited in the presence of adenosine triphosphate (ATP), but significantly enhanced in presence of monophosphates which allows temporal control over dynamic change in protein functionalization via enzymatic ATP hydrolysis. Notably, the NBD-tagging rate towards cysteine and tyrosine residue remains almost unaltered or mildly enhanced in the liquid-like condensed state and shows less pH sensitivity. This work substantiates the alteration in pH-responsiveness of Brønsted basicity of a protein's ε-amine in the condensed phase. Furthermore, this environment sensitivity in catalytic chemoselective protein functionalization in condensed phase will be of importance in adaptable protein engineering to the chemical biology of protein phase separation. Finally, I will share some unpublished data showing enantioselective esterase activity inside protein condensate in a macromolecularly crowded media.

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IL-28

Brief Biography

Subhabrata Maiti

Subhabrata Maiti is currently working as an Assistant Professor at Indian Institute of Science Education and Research (IISER) Mohali. He obtained PhD degree in 2013 from Indian Association for the Cultivation of Science (IACS), Kolkata (supervisor: Prof. Prasanta Kumar Das). Then he moved to University of Padova, Italy to work with Prof. Leonard Prins as a postdoc. In 2017, he did another postdoctoral stint with Prof. Ayusman Sen at Pennsylvania State University (USA) before starting his independent career from October 2018.

He is currently Editorial Advisory Board Member of ChemSystemsChem and Member of the Royal Society of Chemistry (MRSC). In 2024, he was nominated for BIG-ON-SMALL Award in recognition of excellent performance by the International committee of Manipulation, Automation and Robotics at Small Scales (MARSS) at TU Delft, Netherlands.

His present research focus is on exploring chemistry of complex biomolecular systems, emphasizing dynamic (bio)colloidal taxis/phoresis, (bio)catalysis and self-assembly.

IL-29

Catalytic Functionalization of Indole Derivatives Enabled by Iron Complexes

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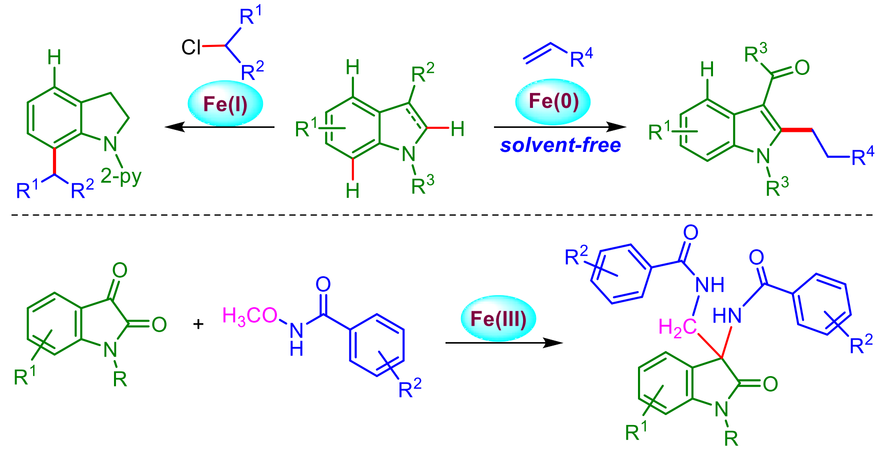
Developing transition metal catalysts based on earth-abundant metals is important to attain sustainable and environmentally benign chemical transformation. In this direction, transition metal catalysts based on iron have been given considerable attention, particularly for the C−H bond functionalization of indoles and derivatives. To this end, our research activities have been focused on the design and development of suitably ligated iron catalysts for selective functionalization of indoles and isatins with the assistance of a monodentate-chelate auxiliary.[1-3] In this presentation, Fe-catalyzed regioselective C–H bond alkylation of indoles and indolines will be discussed. In addition, iron-catalyzed C−C and C−N bond-forming tandem amidation to access the tetrasubstituted 3-amino-3-aminomethyl-2-oxindole frameworks will be highlighted. The focus will be paid to the mechanistic aspects of these reactions. Overall, a comprehensive catalyst development, catalytic scope, and reaction mechanism of the Fe-catalyzed functionalization will be discussed.



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IL-29

Brief Biography

Benudhar Punji

Dr. Punji is a Senior Principal Scientist at the CSIR-National Chemical Laboratory, Pune and a Professor at the Academy of Scientific & Innovative Research (AcSIR), New Delhi. Dr. Punji received Ph.D. from the Indian Institute of Technology Bombay (IITB), Mumbai, under the supervision of Prof. M. S. Balakrishna. Upon graduation, he worked as a post-doctoral fellow with Prof. Alan S. Goldman at the Rutgers University, USA and then as Alexander von Humboldt post-doctoral fellow with Prof Lutz Ackermann at the University of Göttingen, Germany. His research interest includes, development of novel and sustainable 3d transition metal catalysts for C–H functionalizations, asymmetric hydrogenation and (de)hydrogenative transformations. His focus is mostly on mechanistic-based homogeneous catalysis and organometallic chemistry. Dr. Punji has published more than 80 research papers, and he has 10 patents and 8 book chapters to his credit.

IL-30

Development of Mechanically Interlocked Molecules for Targeted Imaging

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NIR emission (650−1000 nm) has benefits in virtue of deep tissue infiltration, minimal background noise, and trivial autofluorescence that proffer a remarkable technique for super-resolution bioimaging. I will show the design of NIR fluorescent mechanically interlocked molecules (MIMs) for selective targeting and real-time tracking of live-cell organelles.[1,2] Dual targeted NIR rotaxane will be demonstrated for living cancer cell-specific active targeting, subsequently selective staining of lysosomes and mitochondria.[2] Single imaging modalities, e.g., USG, CT, PET, SPECT, MRI, and fluorescence imaging, have made enormous curiosities in biomedical science and clinical diagnosis. Each imaging modality has its inherent benefits and limitations concerning sensitivity, penetration depths, resolution, and the risk of exposure to radiation (for CT) and radioactive substances (for PET/SPECT). NIR fluorescence (NIRF) exhibits extraordinary sensitivity at the molecular level with fast response. Yet, NIRF imaging has its intrinsic restriction, e.g., it is incompetent to provide anatomical 3D information. In comparison, MRI exhibits unhindered penetration depth and provides 3D tomography of soft tissues at a higher spatiotemporal resolution than other imaging methods. Nevertheless, MRI displays miserable detection sensitivity and is incompetent at tracking molecular events. A single imaging method is dubious to meet all of the criteria to solve a diagnostic concern and is unable to afford comprehensive information. Integration of NIRF and MRI is advantageous as they don't involve detrimental ionizing radiation and radioactive materials. Nonetheless, most of the NIR dyes frequently suffer from quenching that is a serious concern when they are attached to a magnetic Fe_3O_4 NP-based MR contrast agent. We establish that quenching and photo/chemical bleaching of the dye inside the live-cell and the aggregation of probe complications could be overcome by encapsulating the probe inside a macrocyclic container to develop MIMs that are capped on the Fe_3O_4 NPs. Water-soluble, noncytotoxic MIMs-capped Fe_3O_4 NPs are used for live-cell mitochondria-targeted NIR fluorescence in combination with T_2-weighted MRI with a high relaxation rate (r_2) of 180.7 mM^{-1} s^{-1}.[3] Though the main problem in confocal laser scanning microscopic imaging is the resolution limit of nearly 200 nm that is incompetent to resolve mitochondrial cristae.[3] Stimulated emission depletion (STED) nanoscopy has been revealed as a prevailing imaging device and has the capability to bring a definitive revolt to contemporary bioimaging.[4] A NIR fluorescent MIMs-peptide conjugate will be demonstrated that has been used for live-cell super resolution targeted *STED microscopy.*

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IL-30

Brief Biography

Samit Guha

Dr. Samit Guha currently is an Assistant Professor, Department of Chemistry, Organic Chemistry Section, Jadavpur University, Kolkata.

He obtained his **PhD** from Indian Association for the Cultivation of Science, India (2009).

Postdoc

Florida State University, Florida, USA (2010-2011)

Alexander von Humboldt Fellow, postdoctoral researcher, University of Göttingen, Göttingen, Germany (2011-2013);

University of Notre Dame, Indiana, USA (2014–2015)

Awards: DST-SERB Early Carrier Award (2018), Government of India

Innovator Award (2014) for US patent, USA

Alexander von Humboldt Fellow (2011-2013), Germany.

Current Research Interests: Mechanically Interlocked Molecules, Rotaxanes, Cyanine Dyes, Selective Targeting and Imaging of Cellular Organelles, NIR Organic Biomarkers and Biosensors, Multimodal Imaging Agents, Mitochondria Targeted Chemoselective and Site-Specific Protein Labeling.

IL-31

How Distal is Distal C(sp^3–H) Activation?

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A mild, redox-neutral, transition-metal-free tandem perfluoroalkylation and remote C(sp^3)–H alkylation of terminal alkenes has been achieved through organophotocatalysis, showcasing high chemo- and regioselectivity. This versatile methodology enables difunctionalization at various distances-such as 1,10-, 1,14-, 1,11-, 1,7-, and 1,6-positions-on unactivated alkenes, and highlights a unique radical translocation between secondary C(sp^3) centers with comparable bond dissociation energies. Furthermore, this study introduces a tandem process incorporating trifluoromethylation, 5-exo-trig cyclization, 1,5-radical translocation, and C(sp^3)–H alkylation on 1,6-dialkenes. A key breakthrough is the multi-component, transition-metal-free tandem approach for synthesizing highly substituted cyclopentane derivatives. This sequence involves two consecutive hydrogen atom transfer steps: an initial 1,5-HAT from a secondary to a tertiary C(sp^3) site, followed by a 1,6-HAT from a vinylic to a secondary carbon. The synthetic utility is demonstrated through scalability and subsequent product transformations into valuable functional groups, highlighting the broad applicability and innovative potential of this method.

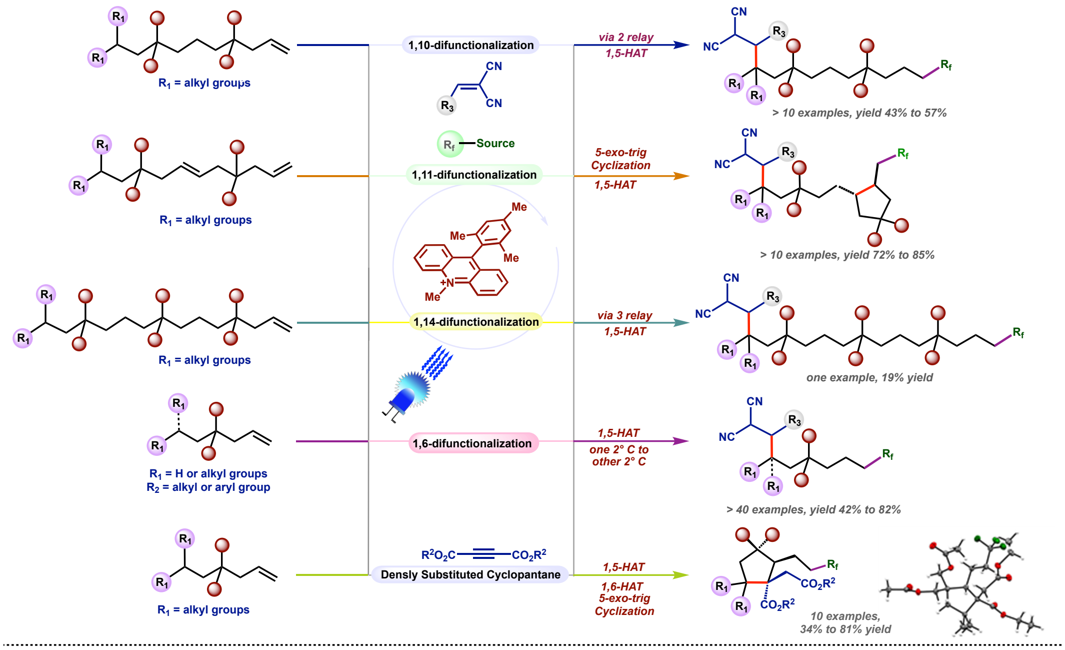

Figure 1. 1,n-Difucntionalization of long chain unactivated alkenes

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IL-31

Brief Biography
Devarajulu Sureshkumar

Career Profile:

Devarajulu Sureshkumar completed his B. Sc. in Chemistry and M. Sc. in Organic Chemistry at the University of Madras. He earned his Ph.D. in 2007 under the supervision of Prof. S. Chandrasekaran, Department of Organic Chemistry, IISc Bangalore. From 2008 to 2010, he was an AvH postdoctoral fellow, working with Dr. Martin Klussman in Prof. Benjamin List's group at the Max-Planck-Institute for Kohlenforschung, Germany. He then undertook a short postdoctoral associate position with Prof. Wilhelm Boland at the Max-Planck-Institute for Chemical Ecology in Jena, Germany, before moving to Japan as a JSPS fellow. There, he worked with Prof. Masakatsu Shibasaki at the Institute of Microbial Chemistry in Tokyo (2010-2015). He joined the IISER Kolkata as a faculty in the Department of Chemical Sciences in February 2015. Currently, his research focuses on visible-light-mediated photocatalysis for C–C bond-breaking and forming and fluorination reactions through C(sp^3)–H functionalization.

Significant Awards/Achievements:

Early Carrier Research Award-2017 from SERB, Government of India.
Ramanujan Fellowship-2016 from SERB/DST, Government of India.
JSPS Fellowship-201 for Foreign Researchers (Pathway to University Positions in Japan).
JSPS Fellowship-2011 at Institute of Microbial Chemistry, Tokyo, Japan.
AvH Fellowship-2008 at Max-Planck Institute for Khölenforschung, Germany.

Representative Publications:

1. Ghosh, K. G.; Pal, K.; Mallick, M.; Das, D.; **Sureshkumar**, **D***. *Adv. Synth. Catal.* **2024**, *Accepted.*
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IL-32

Tuning Piezoelectric Responses in Naphthalene Diimide Appended Peptides and Amino Acids through Controlled Self-Assembly

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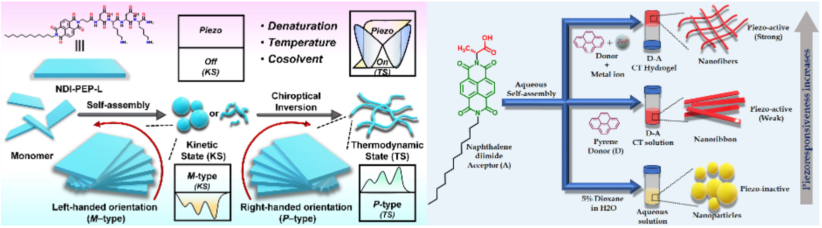
The ability to tailor piezoelectric properties in organic materials through supramolecular self-assembly opens new avenues for creating biocompatible and flexible electronic devices. Recently, we have investigated the self-assembly behavior of naphthalene diimide (NDI)-conjugated peptides and amino acids and its impact on their piezoelectric responses. By tuning the molecular arrangement within these systems, we demonstrate a dynamic modulation of piezoelectric properties, paving the way for innovative material design.

Using a combination of spectroscopic techniques (UV-Vis, PL, FTIR, NMR, CD) and atomic force microscopy (AFM), we explore the self-assembly of NDI-conjugated peptides. A key feature of our findings is the chiroptical switching between kinetically stable nanoparticles and thermodynamically stable nanofibers. This structural transformation is associated with a switchable piezoelectric effect, offering dynamic control over material properties (Scheme1 left panel).[1] In a separate study, we observed that NDI-conjugated amino acids form nanoparticles in aqueous solutions,[2] which exhibit no piezoelectric response. Interestingly, the incorporation of external guest molecules such as pyrene (a donor) transformed these nanostructures into 2D nanoribbons, driven by the formation of a charge transfer (CT) complex between NDI and pyrene, resulting in detectable piezoelectric responses. More strikingly, the further introduction of Zn^{2+} metal ions into the CT complex led to the transformation of the solution into a hydrogel with a crosslinked nanofibrillar structure. This structural change significantly enhanced the piezoelectric response, attributed to the unidirectional alignment of dipoles (Scheme1 right panel). These results demonstrate that by carefully manipulating both molecular interactions and the self-assembly environment, we can achieve a high degree of control over piezoelectric properties in NDI-conjugated systems.

These findings highlight the immense potential of supramolecular self-assembly in tuning the piezoelectric properties of NDI-appended peptide/amino acid-based materials. This strategy offers promising opportunities for the design of functional materials with applications in sensors, actuators, and energy-harvesting devices.



Scheme 1. Schematic representation of controlling piezoelectric responses of NDI-conjugated peptide (left panel) and amino acid (right panel)

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IL-32

Brief Biography

Goutam Ghosh

Experience

Dr. Goutam Ghosh received his Ph.D. in 2014 from the University of Calcutta, Kolkata, India. After completing his Ph.D, he joined the Indian Association for the Cultivation of Science (IACS), Kolkata, in 2015 as a postdoctoral researcher, where he focused on controlled supramolecular polymerization of π-systems and supramolecularly engineered polymers. Subsequently, in 2019, he moved to the University of Münster, Germany, as a postdoctoral research fellow, furthering his expertise in supramolecular chemistry. After returning to India in 2022, he joined the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) as a postdoctoral fellow for a very short time. Currently, Dr. Ghosh holds the Ramanujan Faculty (Assistant Professor) position at the Centre for Nano and Soft Matter Sciences (CeNS), Bengaluru.

Research Summary

Dr. Ghosh's research primarily focuses on the controlled supramolecular polymerization of peptides, amphiphilic molecules, and π-conjugated systems. His work explores their self-assembly behavior and their wide range of applications in fields such as materials science, biomedicine, and energy harvesting. Specifically, he investigates pathway complexity in supramolecular polymerization and the development of functional nanomaterials with tunable properties.

IL-33

Dehydrogenative coupling of alcohols with internal alkynes: An access to β-deuterated branched ketones

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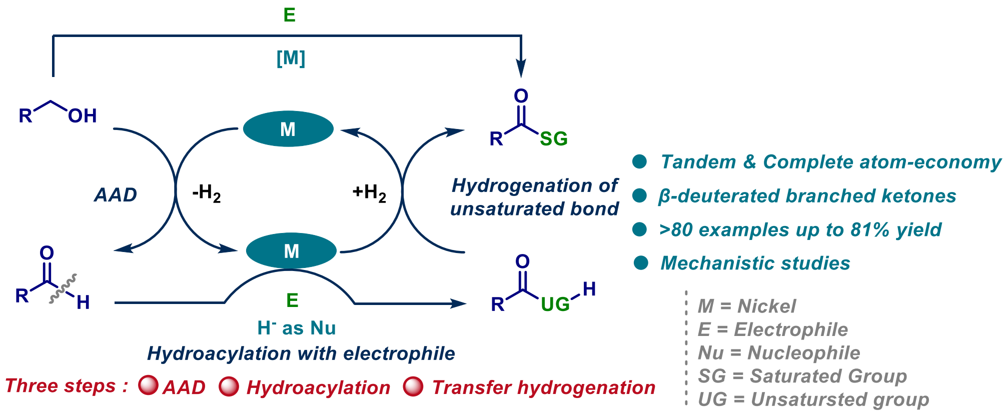
In the realm of synthetic organic chemistry, the pursuit of novel methods for complex chemical synthesis presents both intriguing opportunities and formidable challenges. Traditionally, alcohols serve as alkylating agents in forming C-C and C-N bonds through a dehydrogenative borrowing hydrogen approach in transition-metal catalysis. However, their use as acylating agents in C-C bond formation is notably difficult and infrequently documented. This study introduces the dehydrogenative coupling of benzylic alcohols with internal alkynes under nickel(II) catalysis, employing alcohols as acylating agents. The process yields an array of α-branched aryl ketone derivatives, achieving zero waste via an umpolung borrowing hydrogen technique. Additionally, the study showcases the versatile applications of the resulting α-di-substituted ketones as precursors for other valuable compounds, including the large-scale production of β-deuterated branched ketones. To shed light on the underlying reaction mechanism, a series of spectroscopic analyses, the identification of intermediates, and density functional theory calculations were conducted.



. **Figure 1.** Nickel-catalyzed dehydrogenative coupling of alcohols with internal alkynes

Reference: M. Subaramanian, C. Gouda, Triptesh K. Roy, G. Sivakumar, S. Banerjee, K. Vanka, E. Balaraman*. Dehydrogenative Coupling of Alcohols with Internal Alkynes under Nickel Catalysis: An access to β-deuterated branched ketones. *ACS Catal.* **2024**, *11*, 8294-8309.

IL-33

Brief Biography

Ekambaram Balaraman

Dr. Ekambaram Balaraman received his M.Sc in Chemistry from R.K.M. Vivekananda College, Chennai (2002), and Ph.D from the Central University of Hyderabad (2008). Subsequently, he has been an FGS-Post Doctoral Fellow at the Weizmann Institute of Science (2008-2012). In July 2013, he started his independent career as a senior scientist at the CSIR-National Chemical Laboratory. In Dec'2018, he moved to the IISER-Tirupati as a faculty in chemistry. He is the recipient of the MRSI Medal (2021), SwarnaJayanti Fellowship (2020), CRSI-Bronze Medal (2020), The Asian and Oceanian Photochemistry Association (APA) for Young Scientist (2019), Fellow of Royal Society of Chemistry (2019), AV Rama Rao (AVRA) Young Scientist Award (2018). He is a member of the Indian National Young Academy of Science (INYAS), INSA (2018).

Dr. Balaraman's research primarily focuses on generating resources for green energy and recycling atmospheric waste. Specifically, he works on the design and development of catalytic materials for hydrogen generation from feedstocks, sustainable chemical synthesis, and conversion of CO_2 to value-added products. He is also interested in the development of electron donors for heterogeneous Ziegler catalysts used in the manufacture of isotactic polypropylene.

IL-34

Regulating Spatial Configuration in Donor-π-Acceptor for Through-Space Exciton Transfer: Concentration-Independent Emitter for OLEDs

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Thermally activated delayed fluorescence (TADF) emitters have garnered much attention due to 100% exciton utilization and toxic metal-free design. However, most of the TADF emitters experience a concentration-quenching effect due to which emitting layers are dispersed into the host matrix. There is an urgent need to develop emitters that give the same performance and emission wavelength irrespective of the concentration of emitters. Herein, two TADF emitters (2BPy-*p*TC and 2BPy-*o*TC) are designed and synthesized. For both emitters, the nature and energetics of the lowest excited singlet and triplet together with the extent of through-bond exciton transfer (TBET) and through-space exciton transfer (TSET) are unveiled using reliable quantum-chemical calculations. While 2BPy-*p*TC exhibits pre-dominantly TBET, a greater extent of TSET is found in 2BPy-*o*TC. 2BPy-*p*TC displays blue color with emission maxima at 469 nm while 2BPy-*o*TC exhibits green color with emission maxima at 509 nm in toluene. Both emitters show a low singlet-triplet energy gap (ΔE_{ST}) of 0.20 eV for 2BPy-*p*TC and 0.01 eV for 2BPy-*o*TC and a delayed lifetime of 147.4 µs for 2BPy-*p*TC and 7.4 µs for 2BPy-*o*TC. 2BPy-*p*TC shows EQE_{max} of 12% with an Electroluminescence (EL) peak at 467 nm while 2BPy-*o*TC shows EQE_{max} of 24% with EL maxima of 500 nm. In the case of 2BPy-*p*TC, upon increasing the concentration of the dopant from 5 wt% to 100 wt%, the EL peak experiences a bathochromic shift from 467 to 495 nm and EQE_{max} drops from 12% to 5.5%. On the other hand, 2BPy-*o*TC maintains EQE_{max} of ~24% and EL maxima of 500 nm while increasing the concentration of dopant from 5 wt% to 100 wt%. Hence, 2BPy-*o*TC acts as a universal dopant for both doped and non-doped OLEDs through which the tedious co-deposition process can be avoided.

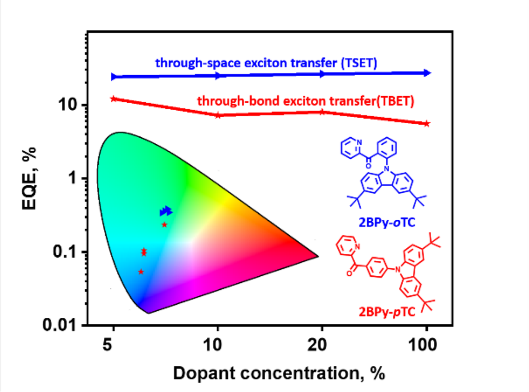

Figure 1. Emitter concentration vs device performance vs CIE values

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IL-34

Brief Biography

P. Rajamalli

RESEARCH EXPERIENCE

2019-present: Assistant Professor, Materials Research Centre, Indian Institute of Science, Bangalore, India
2016-2019: Marie Curie Fellow (Advisor: Prof. Eli Zysman-Colman), School of Chemistry, University of St Andrews, UK.
2012-2016: Post-doctoral fellow (Advisor: Prof. Chien-Hong Cheng), National Tsing Hua University, Taiwan.
2008-2012: Ph.D. in Chemistry (Advisor: Prof. Edamana Prasad), Indian Institute of Technology Madras (IITM), India.

Research summary:

My research group focuses on development emitting materials for organic light emitting diodes (OLEDs) including TADF emitters, carbon, quantum dots and dendrimer derived emitters for solution process. Host and electron transporting materials for highly stable devices. We start with the design of materials, synthesis, photophysical studies and end with device fabrication.

IL-35

Tetravalent Organogermanium/tin Compounds as Catalysts for Organic Reactions

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In recent years, there has been an exploration towards finding new main group catalysts as potential alternatives to transition metal-based catalysts. Main group elements are earth-abundant, less toxic and inexpensive compared to transition metals. Therefore, there is an ongoing development for the synthesis of sustainable and environmentally benign catalysts based on main group elements as alternatives to catalysts of transition metals. Main group catalysts have already been adopted in several organic reactions. In this context, the chemistry of the compounds of group 14 elements has been expanding rapidly. The Lewis acidic nature renders both inorganic and organo-functionalized group 14 elements highly demanding catalysts in organic transformations. Over the last two decades, low-valent group 14 compounds have been extensively investigated and used as catalyst in a wide range of organic reactions. However, they are highly air and moisture sensitive and requires expertise in handling. Interestingly, the catalyst of tetravalent organo-functionalized group 14 catalysts is still developing. In this presentation, we are going to review our efforts to develop new tetravalent organogermanium and organotin compounds as Lewis acid catalyst and their application in organic synthesis.

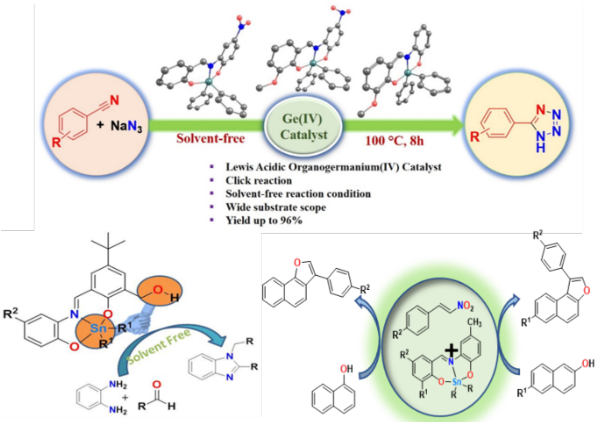

Figure 1. Application of organogermanium/tin(IV) compounds as catalysts in organic synthesis.

Different polydentate ligands have been used to prepare a series of organogermanium(IV) and organotin(IV) compounds. The Lewis acidity of these compounds were determined by standard procedure. All compounds were employed as Lewis acid catalysts in different organic reactions such as Friedel-Crafts Alkylation reaction, [3+2] cycloaddition reaction and in the synthesis of 1,2 disubstituted benzimidazoles. All compounds showed excellent catalytic activities with yield of product up to 92-96%.

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IL-35

Brief Biography

Hari Pada Nayek

Hari Pada Nayek obtained his M.Sc. in Chemistry in 2006 from Indian Institute of Technology Kanpur, India. He received his doctoral degree in 2009 from the Philipps-Universität Marburg, Germany under the supervision of Prof. Dr. Stefanie Dehnen on investigations of the reactivity of bis(trichlorostannyl)organyl compounds. After a postdoctoral stay with Prof. Dr. Peter W. Roesky (2009-2011), he joined as an Assistant Professor in the Department of Chemistry at Indian Institute of Technology (Indian School of Mines) Dhanbad in 2011. Presently, he is working as an Associate Professor. In 2014, he received a DAAD fellowship for a short research stay in the group of Prof. Dr. Stephan Schulz, University of Duisburg-Essen, Germany. He received several research grants from the Science and Engineering Research Board (SERB), CSIR and executed the projects. He has 78 scientific publications. His current research interests include organotin, organogermanium chemistry, lanthanide chemistry and their applications in catalysis.

OP-1

Ru(II)-Catalyzed Macrocyclization via C-H activation to Access Indoline-Braced Metacyclophanes.

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Indole and other heteroaryl motifs are important components of macrocyclic bioactive natural and synthetic compound of therapeutic importance.[1] Compared to their liner counterparts, FDA-approved macrocyclic medications exhibit superior therapeutic qualities.[2] However, to synthesis macrocycles, the current classical methods requires pre-functionalized terminals which needs suitable functional group manipulations and thus limit the scope of the substrates with desired functionality. In this case, cyclization via C-H activation appears to offer a viable resolution.[3] Here, we present the first method of accessing indole-based macrocyclic molecules using Ru-catalyzed cylization. This strategy lead to the synthesis of metacyclophanes with ring size ranging from 13 to 23 members. The pre macrocycles tethered with various ester, amide, ether linkers are well tolerated to generate macrocycles in synthetically good yields. Interestingly, carbohydrate and drug candidates also successfully incorporated as linkers to give a new class of hybrid cyclic structures.

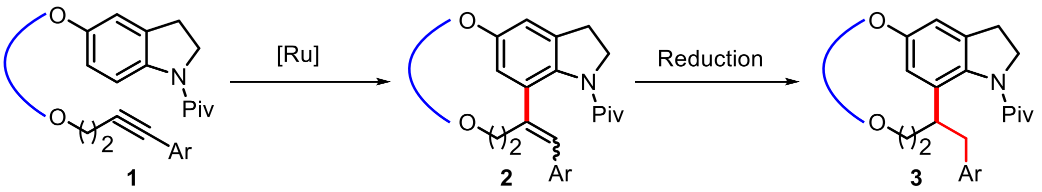

Figure 1. Ru-catalyzed cyclization to access indole grafted macrocyclic compounds.

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OP-2

Design and Characterization of Nickel Complexes as Analogues for Ni_p Sites in Acetyl Coenzyme A Synthase/CO Dehydrogenase: Electrochemical and CO Reactivity Properties

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Primordial life processes stand on carbon-carbon bond formation from prebiotic precursors like carbon dioxide and carbon monoxide.[1] Nickel-containing bifunctional metalloenzyme, carbon monoxide dehydrogenase (CODH)/acetyl coenzyme A synthase (ACS) plays two vital roles namely the reduction of CO_2 to CO (CODH activity) that occurs at the C-cluster of the enzyme and the other is the synthesis of the biological metabolite, acetyl-CoA (ACS activity) that occurs at the A-cluster of the enzyme, utilizing the CO generated from C-cluster, a $–CH_3$ group and the Coenzyme-A thiol.[2,3] The biochemical reactivity of the native enzyme reveals that the acetyl-CoA synthesis takes place at the labile M_p site of the A cluster (represented as M_p site in Scheme-1; M = Ni(II) or Cu(I) or Zn(II)) which has three Cys-S and an unknown ligand (L) coordination to Ni(II). The synthetic models for the Ni_p site are limited. In this poster, we present the synthesis, spectroscopic characterization including X-ray structure of few Ni(II)-thiolate complexes (mono-, bi- and tri-nuclear Ni^{II} complexes such as **1-3** and the hetero bi- and tri-nuclear complexes as **4** and **5** containing the Ni(II)-Cu(I) and Ni-Zn-Ni core respectively) as the model for Ni_p site. The X-ray crystal structure of **2** & **3** reveal a nearly square planar $Ni(II)P_2S_2$ and $Ni(II)S_4$ moiety respectively those may mimic the reactivity of the Ni_p site of ACS. The spectroelectrochemical studies and CO reactivity have been presented in details that may help to understand the mechanism of ACS activity of the enzyme. Generation of Ni(I) species following electrochemical or chemical reduction and subsequent Ni(I)-carbonyl species formation are spectroscopically evident (EPR spectrum of Ni^I species: $g_1 = 2.12$, $g_2 = 2.02$, $g_3 = 2.00$; FTIR of Ni^I-$(CO)_2$ adduct: ν_{CO} = 1934 and 1996 cm^{-1}). Noteworthy, the ν_{CO} of model are comparable to that of the CO-bonded reduced A-cluster that displays the ν_{CO} at 1996 cm^{-1}.

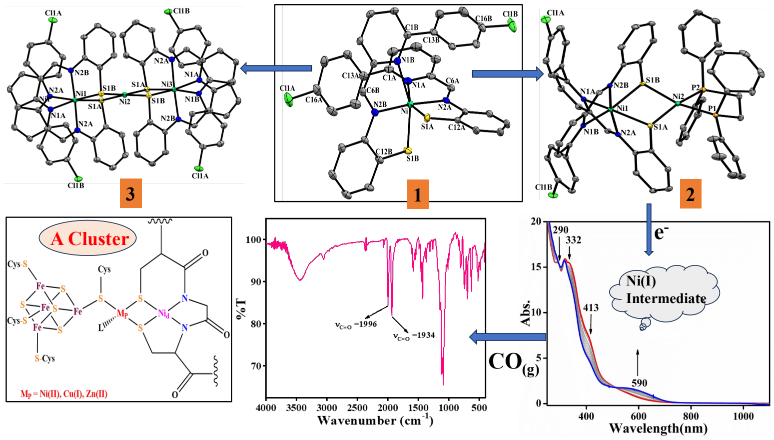

Figure 1. Graphical abstract on nickel complexes as analogues for Ni_p sites and their CO reactivity.

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DECON-impregnated hydrogel-based soft contact lens- a novel approach in inhibiting ocular herpetic inflammation

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Vision loss is attributed to corneal inflammation caused by either viral or non-viral infections [1]. Topical corticosteroids are commonly used drug to treat corneal inflammation, but their efficacy is limited due to the presence of ocular barriers [1, 2]. Moreover, conventional eye drops deliver only 0.07%–4% of the dose to the eye, with most of it being drained through nasolacrimal gland and reflex blinking [3]. Hence, frequent doses at high concentrations are usually advised leading to a reduced patient compliance. Thus, a topical drug delivery system that can overcome the barrier and release drug in a sustained manner while residing in the eye for a longer period is critically needed. In our quest to develop drug delivery platforms, we came across hydrogel-based soft contact lenses for the delivery of ophthalmic drugs [4]. The impregnation of microparticles carrying lipophilic or corticosteroid drugs at their surface was most intriguing. That allows transfer of drug from the concave surface of the contact lens to the cornea through diffusion. It also suggests that the amount of drug absorption to the cornea right just after wearing the contact lens is equivalent to the amount of drug being transferred to the eye after a single drop from conventional eye drops indicating the advantage of using microparticles-integrated contact lenses. Furthermore, the compound activated carbon (black soot) which is a well-known ingredient since ages typically used for the eye was found to improve drug adsorption and penetration topically. It is proven to be nontoxic, cost-effective, and nonimmunogenic in nature [5, 6]. There is a report on improving the efficacy of commercially used anti-viral drug, acyclovir for treating HSV infection when loaded onto the pores of carbon particles termed as drug-encapsulated carbon (DECON) [5]. Herein our current study, we explored microparticles of activated carbon in loading anti-inflammatory drug such as dexamethasone and prednisolone and incorporated into biodegradable hydrogel-based contact lenses made with sodium alginate and Poloxamer. While prednisolone is a commonly used corticosteroid drug and is mostly preferred due to its greater corneal permeability, yet we chose dexamethasone too in our current study to demonstrate that drugs with lower permeation when loaded into DECON -impregnated contact lens can be more effectively delivered to the ocular tissue. Furthermore, dexamethasone is 6-times more potent on a molar basis than prednisolone which will allow our study to deliver lower quantities of total carbon to the eye. We observed that carbon was able to load 96 % of the drug and demonstrated a sustained release over a period of 72 h and interestingly the released drug concentration was higher in presence of HSV virus suggesting a distinctive advantage in drug release. Studies involving murine models of corneal herpes infections demonstrate DECON when administered topically led to a reduced dosing frequency, shortened treatment duration, and improved therapeutic efficacy with a lesser concentration compared to commercially used drugs alone. Additionally, DECON-impregnated contact lenses showed higher efficacy in inhibiting inflammation with just one application. We also show DECON incorporating into a gel-based ointment and eye liner lead to release drug over a period and ultimately inhibit inflammation.

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OP-4

Unveiling the Role of Solvent in Solution Phase Chemical Reactions using Deep Potential-Based Enhanced Sampling Simulations[1]

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Realistic modeling of chemical reactions in the solution phase mimicking experimental conditions has been a challenging task for the simulation community. This is due to the inherent complexity of designing a potential model for a solution-phase multicomponent chemical reaction involving solutes and solvents and the excessive computational resources required to simulate the reaction progress. A way out has been ab initio molecular dynamics (AIMD) simulations that are often considered the gold standard for investigating chemical reactions at the electronic level. A major drawback of AIMD methods is their substantial computational resource requirements. They are not efficiently applicable beyond systems containing approximately a few hundred atoms. Moreover, these methods are limited in their ability to study systems over long time scales, providing only short trajectories of a few picoseconds. In such short time scales, “rare events” such as chemical reactions occurring at milliseconds to seconds with a high TS barrier cannot be simulated. To overcome this, AIMD is often combined with collective variable (CV)-based enhanced sampling (ES) techniques, such as umbrella sampling, metadynamics, and OPES. These methods allow the sampling of metastable states and construction of free energy surfaces (FES) for reactions, but still require long simulation times, often beyond the capabilities of AIMD.

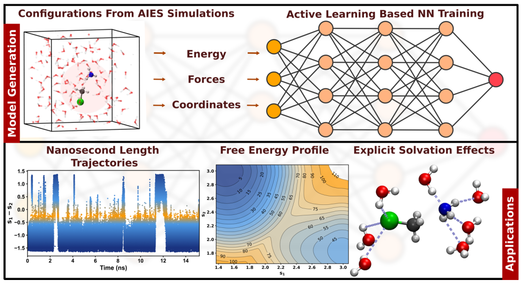

Figure 1. Graphical abstract of the work on use of MLPots for studying chemical reactions

In the pioneering work of Behler and Parrinello, neural network (NN) based machine learning potential (MLPot) has been developed and proposed as a potential solution to address the problem of trade-off between efficiency and accuracy in ab initio methods.[2] MLPots can help us efficiently understand the physics of reactive systems in condensed phases with the accuracy of first principle methods. In our study, we used an active-learning-based deep learning approach to develop an MLPot for solution phase chemical reaction and investigated the effect of solvent on reaction progress. As a prototypical example, we have studied a well-known example of a bimolecular nucleophilic substitution reaction - the Menshutkin reaction, which involves transferring a methyl group to ammonia. This is an interesting yet challenging reaction to model as it involves a transition from neutral reactants (ammonia and chloromethane) to a charged product (methylammonium and chloride) state. Using this MLPot, equilibrium unbiased simulations of the reactant and product states to check the stability of the metastable states. The simulation trajectories were stable for tens of nanoseconds. We also carried out enhanced sampling simulations to sample the reaction process efficiently. Multiple transitions between the reactant and product states allowed us to calculate the converged free energy surface for the reaction. An essential component of our study was to examine the effect of explicit solvents on the reaction. The solvation analysis reveals distinct profile for nitrogen and chloride during the reaction. Nitrogen experiences a steep decrease in solvation before the transition state (TS), Chloride, on the other hand, shows an increase in solvation as it detaches, with hydrogen bonding stabilizing its negative charge in the TS, facilitating the reaction. This highlights that solvation and desolvation occur differently for nitrogen and chloride, particularly around the TS. Our approach expands the scope of studying the chemical reaction under realistic conditions, such as explicit solvents at finite temperatures, closely mimicking experiments.

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OP-5

Metal-Ligand Cooperation and Redox Promoted Alcohol Activation Using Zinc Complex

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Inspired by nature's redox management in bioinorganic systems, [1] we developed various Zn-complexes to catalyze radical-mediated [2] borrowing hydrogen process for producing β-disubstituted ketones. A diverse range of secondary alcohols, including fatty alcohols, terpenoid and steroid analogues, were successfully utilized for the chemo-selective functionalization of ketones. Hydrogen atom transfer (HAT) relay the dehydrogenation of alcohols and control experiments incorporating deuterium labelling to the alcohol acclaimed the borrowing hydrogen (BH) pathway for the catalytic cycle. Radical quenching experiment endorse the radical pathway in catalytic cycle. Kinetic study underpins the first order reaction profile was followed with respect to both the starting materials. A thorough mechanistic study reveal that base mediated N-H abstraction initiate the metal-ligand cooperation (MLC) *via* dehydrobromination, followed by $1e^-$ reduction produce the active catalyst.[3]

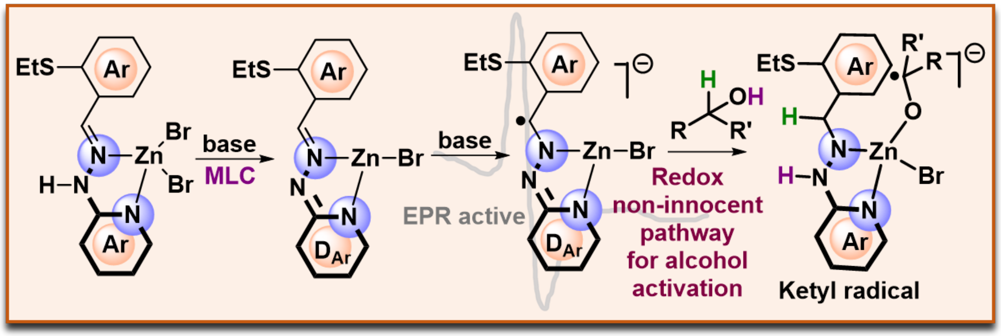

Figure 1. Graphical abstract of synergistic MLC and Redox enabled alcohol activation.

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OP-6

Fe(III)-Complex Incorporated and Surface-Modified Porous Silica Nanosphere as Hepatocyte-Targeted MRI Contrast Agent

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Magnetic resonance imaging (MRI) is one of the most potent non-invasive diagnostic imaging modalities that provides high-resolution 3D images of soft tissues without using harmful ionizing radiations, such as those used for X-rays, computerized tomography, *etc.*[1] To enhance the sensitivity of MRI scans and improve the visibility of healthy and diseased tissues, contrast agents, which are usually small complex molecules of Gd(III) ion, are often utilized. Herein, to explore more bio-friendly metal ions as the constitute of the contrast agent,[2] we have synthesized a six-coordinated Fe(III) complex, Complex **1**, with excellent thermodynamic stability (log $K_{\text{cond}} = 23.6$). However, it demonstrated low relaxivity ($r_1 = 0.59$ mM^{-1}s^{-1} at 37 °C, pH 7.4) due to the absence of inner-sphere water molecules.[3] Thus, limiting its effectiveness as a small molecule-based MRI contrast agent. To overcome this limitation, Complex **1** was encapsulated into porous silica nanospheres, and further surface modifications were implemented using 3-aminopropyltriethoxysilane (APTES) followed by paramethoxybenzoate (PMBA) units to introduce positive charge and hydrophobicity on the nanoparticle surface. The alteration resulted in **C1**@SiO_2-PMBA-NP, which aimed to facilitate targeting hepatocytes for liver-specific contrast enhancement. Indeed, the integration of Complex **1** into the silica nanospheres led to a significant improvement in longitudinal relaxivity r_1 to 5.36 mM^{-1}s^{-1}. The effectiveness of the surface-bound PMBA unit on the synthesized nanoparticle was established through fluorescent imaging of HepG2 cells, demonstrating the efficient uptake of the nanoparticles by hepatocytes when compared with the nanoparticle without the PMBA group. Furthermore, *in vivo* studies using C57BL/6 mice aided the potential of **C1**@SiO_2-PMBA-NP as a liver-targeted T_1-weighted MRI contrast agent, indicating its promise for hepatocyte-specific imaging applications.

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OP-7

$Sc(OTf)_3$-Catalyzed Domino *C–C/C–N* Bond Formation of Aziridines with Quinones *via* Radical Pathway

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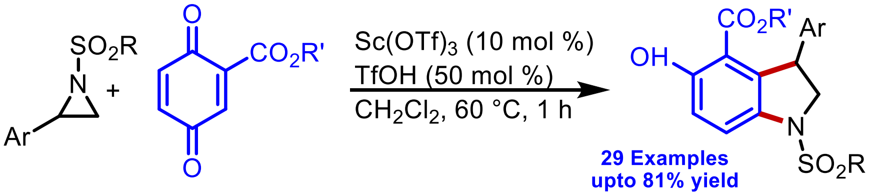
An efficient and attractive methodology has been developed for the preparation of substituted indoline moieties employing aziridines and quinone esters. A Sc(III)-catalyzed one-pot domino *C-C/C-N* bond formation procedure provides a potential route for synthesizing substituted indoline moieties with functional group diversity. The umpolung reactivity of aziridines, radical pathway, mild reaction condition, substrate scope and coupling of drug molecules in post-synthetic application are the essential practical features.[1]



♦ Access to Indoline ♦ Radical Pathway ♦ Substrate Scope ♦ Mild Condition

♦ Cascade *C-C/C-N* Bond Formation

Figure: Sc(III)-catalyzed unprecedented (3+2) cycloaddition of aziridines with quinone esters

Reference

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OP-8

Magnetic Nanoparticles as Magnetic Hyperthermia Agents

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Magnetic nanoparticles (MNPs) find wide applications in various fields due to their magnetic properties, ease of separation, cytocompatibility, and high surface area-to-volume ratio. Cancer therapy being one of the biomedical applications, in which MNPs are used as heat mediators for thermal therapy of cancer cells. MNPs based thermal therapy of cancer cells is generally termed as "Magnetic Hyperthermia" (MHT). Briefly, MNPs formulation is injected into patient's body and is directed towards the tumour mass where, in presence of an externally applied alternating magnetic field (AMF) these NPs generate heat in order to ablate cancer cells. A temperature range of 40-45 °C is referred as the hyperthermia range. However, there are a few practical constraints in their biomedical application such as, low biocompatibility for longer exposure and poor colloidal stability. Doping remains a simple approach for tuning their physical properties whereas, surface modification improves their chemical characteristics. In the present work, we have synthesized zinc doped cobalt ferrites for their application in hyperthermia treatment for cancer therapy. The nanoformulation can be expressed as Zn_xCo_{1-x}Fe2O4. Dopant amount was varied from x = 0-1 (M), with an interval of 0.2. Co-precipitation synthesis was employed to obtain the aforementioned NPs. Afterwards, the obtained NPs were calcined at 800 °C for 4 h to obtain the pure phases. Characterization techniques such as, Fourier Transform Infrared spectroscopy (FTIR), X-Ray Diffraction (XRD), X-Ray Photoelectron Spectroscopy (XPS), Vibrating Sample Magnetometer (VSM) measurement were used to characterize the prepared NPs. These NPs were also analysed for their cytocompatibility using HEK293 cells and antibacterial potential against both, gram-positive (Staphylococcus aureus) and gram-negative (*Escherichia coli*) bacteria at various concentrations. All the synthesized NPs were found to be biocompatible even at high concentration of 1 mg/mL for 72 h besides, were also found to inhibit bacterial growth upto 50%. Their hyperthermic potential was analysed against normal body cells (HEK293) and Lung carcinoma (A549) cells where, 50% of cancerous cell reduction was observed for 30 min of hyperthermic treatment sparing the normal cells. Moreover, to improve the colloidal stability of MNPs various chemical and polymeric entities were employed. The surface modified MNPs were then characterized using various analytical techniques and were found to be stable for atleast 2 months at room temperature.

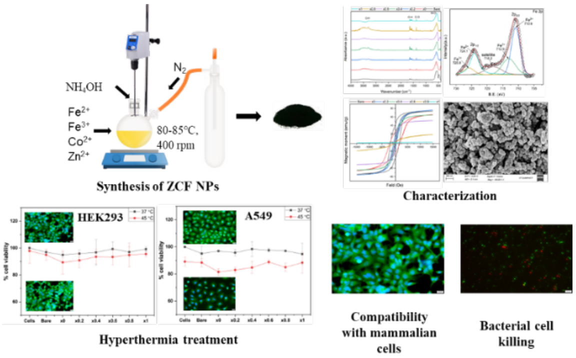

Figure 1. Graphical abstract of the synthesised MNPs and their application as MHT agent.

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OP-9

Photocatalytic, Intermolecular Olefin Alkylcarbofunctionalization Triggered by Haloalkyl Radical Generated *via* Halogen Atom Transfer

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A visible light mediated, haloalkyl radical initiated, three-component olefin difunctionalization is reported. The application of haloalkyl radicals generated *via* halogen atom abstraction by α-aminoalkyl radicals has been demonstrated for accessing a new halogenated chemical space. Overall, the alkylcarbofunctionalization of styrenes was accomplished by employing them as (poly)haloalkyl radical acceptors and subsequent C-C bond formation with quinoxalinones.

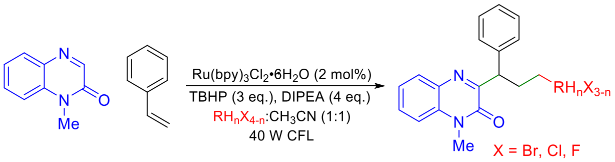

Figure 1. Photochemical haloalkylative olefin difunctionalization *via* XAT

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OP-10

Biopolymer Derived Carbon Dots as a Dual Probe for Delivery of Therapeutics and Vitamin Detection

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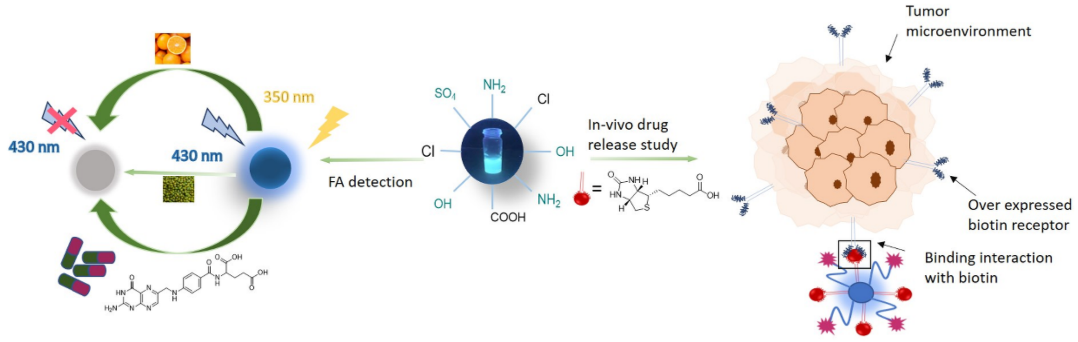
Cancer is one of the most prevalent and lethal diseases worldwide, demanding effective solutions for early diagnosis and targeted drug delivery. Chemotherapy, though a standard treatment, often suffers from low bioavailability and the unintended destruction of healthy cells, leading to severe side effects.[1] Nanomaterials, especially carbon dots (CDs), offer immense potential in cancer diagnosis and treatment, providing advantages such as diverse biomodification, enhanced cellular penetration, and efficient biodistribution.[2] Due to their nano-scale size, CDs can potentially improve the transport of therapeutic molecules to specific tissues, ensuring deep penetration into tumours. The surface functional groups on CDs further play a crucial role in allowing the attachment of drug-targeting moieties via covalent bonding and interactions. In our study, we covalently attached biotin to CDs to increase target specificity. This modification led to significantly higher cellular uptake of the drug in HeLa (cervical cancer) and MDA-MB-231 (triple-negative breast cancer) cell lines, while showing minimal cytotoxicity towards HEK (human embryonic kidney) cells, highlighting the safety profile of the nanocarrier in non-cancerous cells. The internalization and efficacy of these biotin-conjugated CDs were confirmed through bioimaging studies, where the enhanced uptake in cancerous cells (HeLa and MDA-MB-231) was clearly observed. These findings demonstrate the promising potential of CDs in selective cancer treatment, offering both efficacy in drug delivery and minimal impact on healthy tissues.



Scheme 1. Illustration of CD as dual probe for selective detection and targeted drug delivery.

Utilizing the fluorescence properties of carbon dots (CDs), we developed a nanosensor for detecting folic acid (FA) in aqueous systems. FA, a vital vitamin involved in the metabolism process, plays a crucial role in cell growth. However, excessive intake can lead to severe health disorders, including cancer and neural tube defects during pregnancy.[3] Moreover, excess FA excretion into the environment poses risks to living organisms. Thus, monitoring FA levels is critical. In this study, our nitrogen-rich CDs demonstrated high sensitivity in detecting FA, with a detection limit as low as 40 nM, even in the presence of 35 common coexisting analytes. This detection is possible across a broad pH range and has been successfully tested in real samples such as green gram dal and orange extract. These results highlight the potential of CDs not only in targeted drug delivery but also as effective biosensors for monitoring essential biomolecules, offering both environmental and clinical applications (Scheme 1).[4]

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OP-11

Conformational control of Thiourea and Squaramides for ON/OFF Catalysis Regulation

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Switchable catalysis[1] has recently attracted significant interest in supramolecular chemistry due to its similarity to biological catalytic processes that operate under controlled conditions. A switchable catalyst allows modulation of catalytic activity and enables multiple reactions to occur simultaneously in the same reaction vessel, effectively creating an invisible compartmentalization of reaction pathways. Squaramides and thioureas are particularly intriguing compounds in this field because of their strong bidirectional hydrogen bonding capabilities, which has spurred extensive research into their applications in material science and biology.[2] Both squaramides and thioureas serve as organocatalysts through their hydrogen bond donor properties.[3] In this work, we have designed two switchable catalysts by integrating thiourea[i] and squaramide[4] groups with phenanthroline units. This structure allows us to control hydrogen bond donor availability by adding or removing copper(I) ions as a stimulus. In the absence of copper(I), the catalyst adopts an anti-anti conformation, enabling catalytic activity (e.g., for Michael addition). Upon addition of copper(I), the conformation shifts to syn-anti, effectively shutting down catalysis. This reversible switching mechanism was successfully tested over three cycles, showing no decrease in catalytic activity.

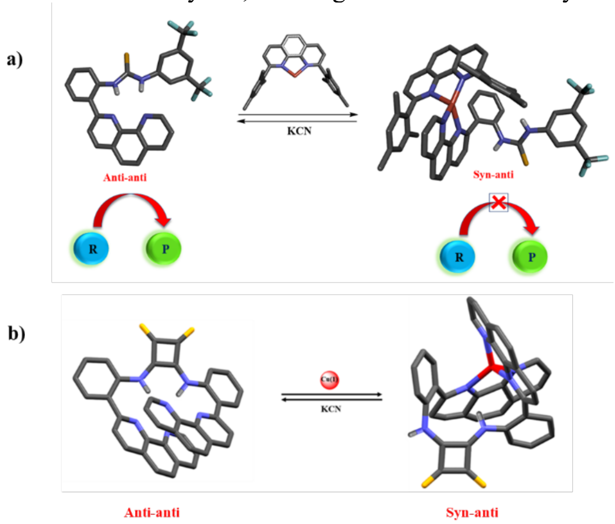

Figure 1. Schematic representation of reversible switching of a) thiourea; b) squaramide based catalysts via metallic stimuli.

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OP-12

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

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Phytic acid (PA) in grains and uric acid (UA), linked to conditions like gout, are important for health monitoring. PA reduces mineral bioavailability and can lower serum uric acid levels. Current fluorescent sensors for PA have slow responses and poor selectivity. Therefore, we designed an AIE-active bisindolyl probe to differentiate PA and UA using hydrogen bonding, aggregation, and electrostatic interactions. This approach leverages photophysical changes in π-conjugated molecular aggregates, enhancing selectivity and sensitivity. Multipoint interactions, especially hydrogen bonding via OH, NH, or positively charged groups, help form stable, stimuli-responsive supramolecular assemblies, improving biosensing applications.

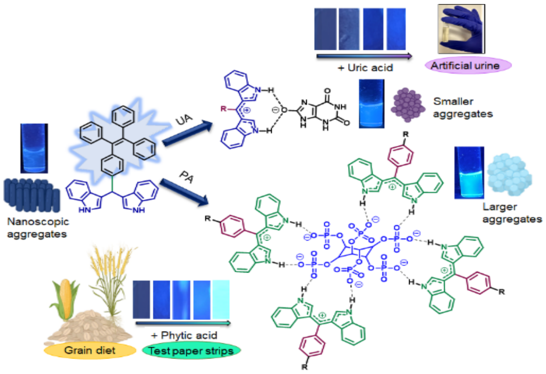

Figure 1. The amphiphilic probe demonstrated selective fluorescence responses to uric acid and phytic acid, and convenient on-site monitoring using pre-coated paper strips.

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

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OP-13

Esterase-responsive Fluorogenic Prodrugs of Aldose Reductase Inhibitor Epalrestat: An Innovative Strategy towards Enhanced Anticancer Activity

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In addition to the conventional chemotherapeutic drugs, potent inhibitors of key enzymes that are differentially overexpressed in cancer cells and associated with its progression are often considered as drugs of choice for treating cancer. Aldose reductase (AR), which is primarily associated with the complications of diabetes, is known to be closely related to the development of cancer and drug resistance.[1] Epalrestat (EPA), an FDA-approved drug, is a potent inhibitor of AR and exhibits anticancer activity.[2] However, its poor pharmacokinetic properties limit its bioavailability and therapeutic benefits.[3] We report herein the first examples of the esterase-responsive turn-on fluorogenic prodrugs **RM-13** and **RM-28** for the sustained release of EPA to the cancer cells with turn-on fluorescence readout.[4]

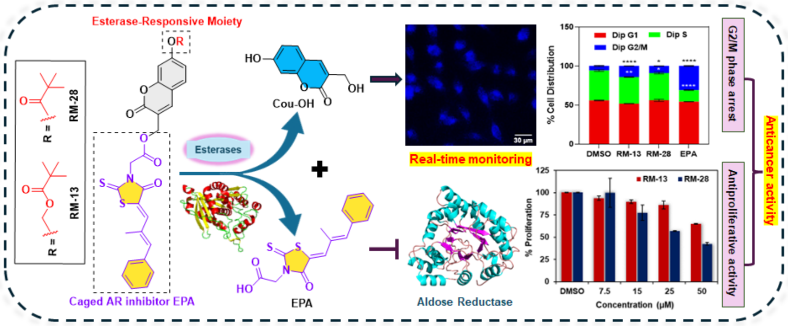

Figure 1. Graphical abstract representing the activation of **RM-13** and **RM-28** in the presence of esterase with concomitant turn-on fluorescence.

The prodrugs could be activated in the presence of esterases, which are overexpressed in cancer cells. Spectroscopic and HPLC studies revealed a simultaneous release of both the active drug and the fluorophore from the prodrugs over time. While the inhibitory potential of EPA released from the prodrugs towards the enzyme AR was validated in the aqueous medium, the anticancer activity of the prodrugs was studied in a representative cervical cancer cell line (HeLa). Interestingly, our results revealed that the development of the prodrugs can significantly enhance the anticancer potential of EPA. Finally, the drug uncaging process from the prodrugs by the intracellular esterases was studied in the cellular medium by measuring the turn-on fluorescence using fluorescence microscopy. Therefore, the present study highlights the rational development of the fluorogenic prodrugs of EPA, which will help enhance its anticancer potential of EPA with better therapeutic potential.

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OP-14

Tripodal AIE active acylhydrazone based probe for selective turn on response towards Zn^{2+} in HEPES buffer and as anion/metal responsive organogelator

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Self-assembly, a nature inspired process leading to the formation of highly functional complex macromolecular systems, utilizing supramolecular interactions from monomeric building blocks, which are crucial for life. Self-aggregated functional systems are promising for drug delivery, development of optoelectronic devices, environmental remediation, and detection of important analytes via fast response to external stimuli. Although the commonly observed aggregation-caused quenching (ACQ) of organic luminophores limits their practical applications, the emergence of aggregation-induced emission (AIE) phenomena by Tang's research team in 20015 has enabled one to utilize the aggregation process to foster light emission. Over the last two decades, the evolution of supramolecular self-assembled systems and the development of sensing strategies have facilitated the creation of excellent multifunctional sensing platforms for sensing metal cations, anions, neutral molecules, etc. Moreover, the molecular self-assembly leading to supramolecular gel formation by specific low-molecular-weight gelators (LMWGs) have drawn immense research interest in recent years owing to their promising applications in diverse areas like chemosensors, drug delivery, biomaterials, biosensors, tissue engineering, hybrid functional materials, etc.

Figure 1. Graphical abstract of the **TRI-QUI** probe showing gelation, AIE and sensing properties.

we have synthesized two acylhydrazone-based probes, **TRI-QUI** and **TRI-NAP**, containing quinoline and naphthalene at their periphery, respectively. **TRI-QUI** responds selectively to Zn^{2+} in 0.1M HEPES, with an LOD value of 6.45 µM. Additionally, **TRI-QUI** can form a stable supramolecular gel in a DMSO: H_2O (2:3 v/v) solution through interconnected network formation driven by H-bonding and π–π stacking interactions. The gelator can also interact with anions and metal cations in the gel phase. Notably, the **TRI-QUI** gel can adsorb small molecules like methyl orange and bromophenol blue, with an uptake efficiency of 63% and 60%, respectively. This work opens the door for developing a multifunctional probe useful for sensing harmful metal ions in solution and creating soft materials applicable in real-life scenarios.

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OP-15

Flexible PVDF-BST Electrospun Nanocomposites for Enhanced Piezoelectric Energy Harvesting

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Abstract

Researchers are working to improve eco-friendly energy and power conversion methods for sustainable development in response to rising concerns about energy security and ecological pollution due to the depletion of non-renewable energy sources [1-3]. In this context, piezoelectric materials stand out for their ability to efficiently harvest energy from environmental sources, such as human activities, to power consumer devices and nanostructures [4-6]. However, flexibility and cost-effectiveness are equally crucial factors for these energy-harvesting technologies. Polyvinylidene fluoride (PVDF) combined with piezoelectric ceramic-based nanocomposites shows great promise for micro-energy harvesting applications [7-9]. This investigation primarily focuses on the synthesis, characterization, and development of a piezoelectric barium strontium titanate (BST)-doped PVDF piezoelectric nanogenerator (PENG) via electrospinning. Firstly, tetragonal-phase $Ba_{(1-x)}\,Sr_{(x)}TiO_3$ (BST) particles were dispersed in a PVDF solution, followed by electrospinning to fabricate the PENG. The PVDF nanofibrous mat loaded with 50 wt% BST produced a nearly thirteenfold increase in output voltage compared to the pristine PVDF nanofiber mat. The study also explores the functionality of the fabricated PVDF-BST PENG by lighting LEDs, highlighting its potential as a promising candidate for flexible and cost-effective energy-harvesting technologies.

Keywords: Piezoelectricity, Electrospinning, Nanocomposite fiber, Energy harvesting

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OP-16

Triphenylamine based CMPs as efficacious photocatalysts towards phenol production, simultaneous detection and degradation of micropollutants

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Herein, we present a detailed insight on the photocatalytic activity of functional materials starting from donor-acceptor conjugated microporous polymers (CMPs) to donor-donor CMPs from some of our recent works. Two donor-acceptor CMPs, namely **PTPA-AQ** and **PTPA-AM** were synthesized *via* Suzuki-Miyuara cross-coupling polymerization. They were facilitated with island like morphology and superior thermal endurance upto 374 ^{0}C. Interestingly, these polymers could exhibit visible light driven superoxide generation which bestowed their application as potential photocatalyst for oxidative hydroxylation of phenyl boronic acid into phenol with 96% yield. To our delight, PTPA-AQ could be recycled upto four successive runs without losing its structural property and photocatalytic efficiency. The efficient intramolecular charge transfer for D-A CMPs insisted us to work diligently on donor-donor CMPs namely, **PTPA-AN-2,6** and **PTPA-AN-9,10**. As evident form their structures, **PTPA-AN-9,10** possessed lesser degree of conjugation resulting into strong cyan fluorescence with characteristic emission maxima at 428 nm. This property was well utilized for detection of picric acid with LOD = 34 μM (Figure 1). On the other hand, the regioisomeric polymer **PTPA-AN-2,6,** having higher degree of conjugation, showed superior activity in visible light driven ROS generation(superoxide). This polymer could efficiently catalyze the reduction of nitrophenol derivatives and superoxide mediated degradation of Congo red with $k = 0.047\ \text{min}^{-1}$ and TOF = $0.024\ \text{h}^{-1}$.[1]

Figure 1. **Triphenylamine Anthracene based CMPs in photocatalytic micropollutant degradation**

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OP-17

MXene derived metal organic framework@PANI heterostructure as a hybrid supercapacitor

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As global challenges of environmental pollution and fossil fuel depletion intensify, the development of sustainable energy storage technologies is crucial [1]. In this context, supercapacitors have gained attention for their long cycle life and high-power density [2]. Metal-organic frameworks (MOFs) are emerging as promising electrode materials for supercapacitors due to their unique physical properties, including high porosity, controllable pore sizes, and abundant active sites. These characteristics enhance ion transport and charge storage, making MOFs attractive for energy applications [3]. However, traditional synthesis methods often struggle with dimensionality control, which can adversely affect electrical conductivity and electrochemical performance.

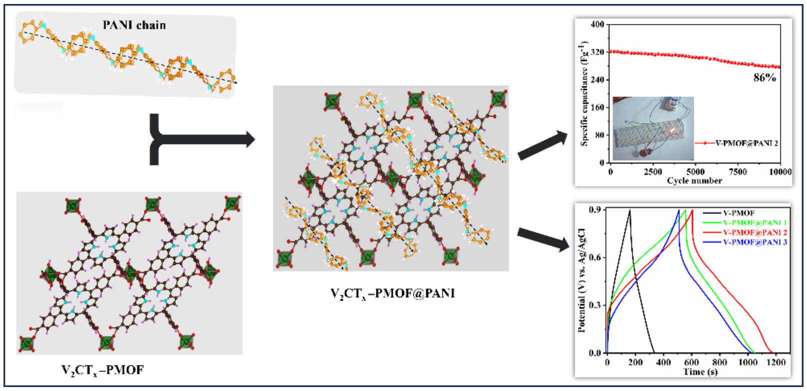

Figure 1. Graphical abstract of supercapacitive performances of V-PMOF@PANI

This study explores the use of V_2CT_x MXene as a novel metal precursor to synthesize two-dimensional (2D) porphyrinic V-PMOF nanosheets using tetrakis (4-carboxyphenyl) porphyrin (TCPP). The resulting V-PMOF demonstrated a specific capacitance of approximately 97 Fg^{-1} at a current density of 0.5 Ag^{-1}. To further enhance performance, a composite material, VPMOF@PANI, was created by integrating polyaniline (PANI) nanofibers onto the V-PMOF sheets. This composite exhibited a remarkable specific capacitance of 322 Fg^{-1} at a current density of 0.5 Ag^{-1} and excellent cyclic stability, retaining 86% capacitance after 10,000 cycles at a current density of 5 Ag^{-1}. These findings indicate that MXene-based MOFs, particularly the V-PMOF@PANI composite, hold significant potential for advancing supercapacitor technology.

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OP-18

A CO_2 Capture Journey through Computational Modeling – Amines and beyond

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Absorbent materials which can separate and capture post-combustion CO_2 have been widely developed and examined in recent times [1,2]. Among various materials available for carbon capture, we present four of our works starting with amino group as a potential CO_2 capture functionality and gradually shift towards amino acids and carboxylates for sustainable CO_2 capture. Firstly, ions of several under-explored isomers of dihydrooxazole family, such as the anions generated from oxazoline, oxadiazoline and oxatriazoline have been investigated quantum chemically as potential azolate based CO_2 capture systems. In the second study, we used quantum chemical methods to determine possible pathways (carbamate *vs*. bicarbonate) for the reactions between CO_2 and various positional isomers of methylpiperidines (N-methyl, 2-methyl, 3-methyl, 4-methyl and their conformational variations, *cis-trans*/*ax-eq*). In the third part of the study, we investigated CO_2 absorption in the aqueous solutions of the potassium salt of lysine amino acid (potassium lysinate, LysK). Understanding the complexity pertaining to the structure, absorption behaviour and dynamics of CO_2 absorption in aq. LysK-CO_2 system using molecular dynamics (MD) simulations, forms the basis of this work. The journey concludes with the investigation of citrate as an anion of non-toxic and biocompatible origin for CO_2 capture as citrate-based ionic liquids (ILs) were found to be easily recycled, non-polluting, less corrosive and easy to synthesize. This forms a crucial step to develop sustainable CO_2 capture process through ILs.

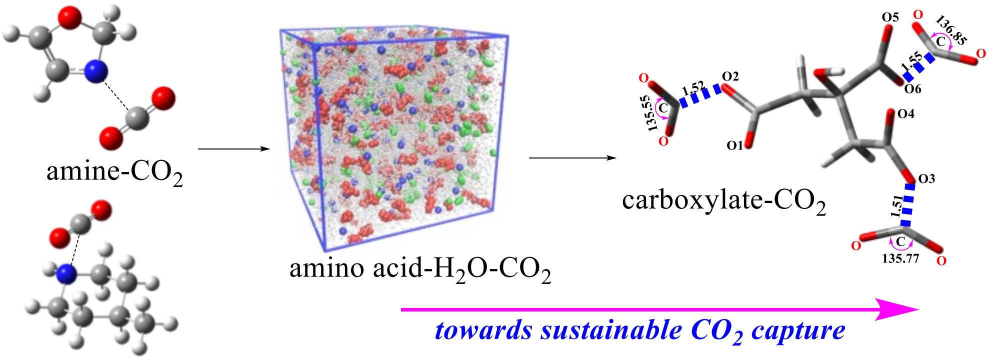

Figure 1. Graphical abstract of the absorbents for CO_2 capture explored and presented in this work.

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IndL-1

An Introduction to Magritek's Spinsolve Benchtop NMR: Its Applications, From Academia to Industries

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Nuclear Magnetic Resonance (NMR) spectroscopy is an indispensable tool for atomistic structural characterization. Since its discovery in the late 1950s, NMR has been extensively utilized in both academia and industry to elucidate complex molecular structures and understand their functional implications. Traditional NMR spectroscopy relies on superconducting magnets, which require ultra-low temperatures to operate, thereby increasing operational costs.

In contrast, Magritek's Spinsolve Benchtop NMR employs a permanent magnet based on the Halbach design [1], eliminating the need for ultra-cool conditions. This innovation significantly reduces costs and enhances accessibility for a broader range of academic and industrial applications. Spinsolve NMR has demonstrated versatility across various fields, from material sciences to forensic science. In industrial settings, it serves as a robust qualitative and quantitative analytical tool, often integrated with other analytical techniques such as High-Performance Liquid Chromatography (HPLC) and reaction monitoring systems [2,3], thereby advancing research and development efforts.

The presentation will explore the scope and potential of Spinsolve Benchtop NMR, highlighting its applications and benefits in contemporary scientific research and industrial practices.

Figure 1: Cryogen free Magritek's Spinsolve Benchtop NMR.

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IndL-1

Brief Biography
Subhendu Pandit

Analytical, organized and well oriented science professional with more than 9 years of research experience in diverse fields from Biochemistry to Biophysics. Always curious to learn and face new challenges. I have a huge apprehension for life and healthy work ethics.

EXPERIENCE
Jun 2023 - Present
PRODUCT SPECIALIST- NMR | Labindia Analytical Instruments Pvt. Ltd**.**
Key Responsibilities: Installation and Application support for Magritek's Spinsolve Benchtop NMR. Developing new NMR methods to address different scientific problems. Application Support for Thermo Fisher's FTIR spectrometer**.**

EDUCATION
Aug 2023
Doctor of Philosophy in Chemistry | TATA Institute of Fundamental Research
- Ph. D Thesis on "Studying Dynamics of Protein Using Solution NMR Spectroscopy"

Sep 2022
Master of Science in Chemistry awarded (Int. Ph. D Course) | TATA Institute of Fundamental Research
- Master Thesis on "Effect of the L99A Cavity Creating Mutant on the Backbone Flexibility of T4 Lysozyme"

Jun 2014
Bachelor of Science with Chemistry (H) | Vidyasagar University
- Topped in College across all subjects.
- DST INSPIRE fellow**.**

SKILLS
- Solution NMR Spectroscopy
- Molecular Biology (DNA Recombinant technology)
- Python, MATLAB programming languages
- Software: Mnova, Topspin, Sparky, NMRPipe, PINT, Sparky, Chimera, GNU Plot, Microsoft office
- FTIR
- Structural Characterization of Protein and other organic molecules using solution NMR Spectroscopy.
- Exceptional communication
- Fluent in English, Hindi, and Bengali

P-1

Superhydrophobic Metal–Organic Framework-Based Composite Featuring Removal of Hydrophobic Drugs and Pesticides and Antibacterial Activities

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The widespread use and contamination of natural sources by new-generation drugs and pesticides have enhanced concern about environmental pollution. Understanding the above importance, we developed a superhydrophobic metal–organic framework (MOF) (**SHMOF′**: $[Zr_6O_4(OH)_4(BDC\text{-}NH\text{–}CO\text{-}R)_{2.4}(BDC\text{-}NH_2)_{0.6}(CF_3COO)_6]\cdot 2.5H_2O\cdot 4DMF$) for ecological remediation via adsorption-based separation of hydrophobic drugs (flurbiprofen) and pesticides (fluazinam). The newly developed **SHMOF′** has a high adsorption capacity toward flurbiprofen and fluazinam, i.e., 435 and 575 mg/g, respectively. The adsorption equilibrium time of the MOF is very short (15 and 10 min for flurbiprofen and fluazinam, respectively). The outstanding superhydrophobic nature of the MOF was employed to separate flurbiprofen and fluazinam from highly alkaline and acidic media and environmental water samples. The **SHMOF′** has excellent selectivity toward the adsorption-based separation of flurbiprofen and fluazinam in the coexistence of common analytes. Again, we developed a polypropylene (PP) fabric-based composite of **SHMOF′** (**SHMOF′@PP**) to separate the hydrophobic targeted analytes by using a zero-energy-consuming filtration-based separation method, which made this separation process cost-efficient and user-friendly. Moreover, Ag nanoparticles were doped to the superhydrophobic composite. The Ag-doped reusable **SHMOF′@PP@Ag** composite exhibited excellent bacterial antiadhesion and antibacterial properties toward *Staphylococcus aureus* bacteria.

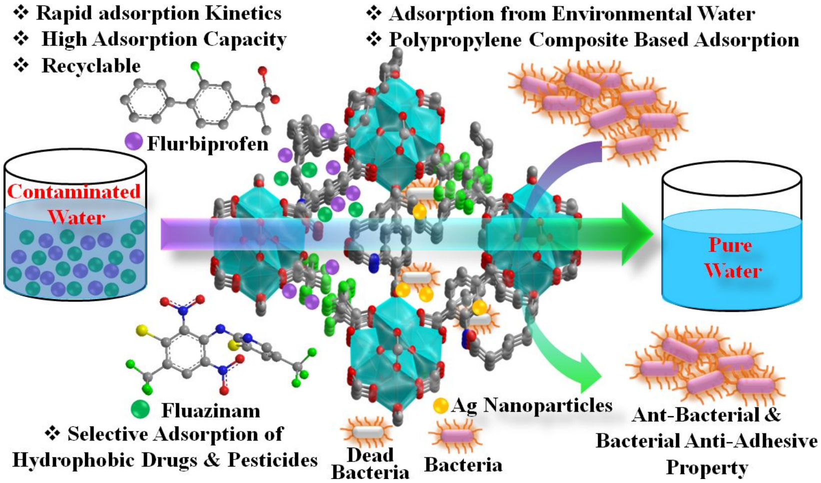

Figure 1. Details of the adsorption-based separation of flurbiprofen and fluazinam by **SHMOF′** and antibacterial property of **SHMOF′.**

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P-2

Microstructural analysis of reverse ATRP-prepared poly (butyl acrylate) grafted silicone rubber using various modes of NMR

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NMR spectroscopy is used to determine the microstructures, sequential distribution of repeating units, and tacticity of a polymer. The chain configuration and bonding alignment of the polymers influence the chemical shift of the NMR signals. Thus, this can be exploited to obtain insight information about the micro-structures present in a polymer. This study presents the synthesis of poly(butyl acrylate) grafted silicone rubber (MQ-*g*-PBA) via reverse atom transfer radical polymerization (RATRP) and their structural characterizations. The structural characterization of this prepared graft copolymer was carried out using various analytical techniques such as FT-IR, UV-Vis and NMR. However, NMR was extensively used to investigate various microstructures present in the grafted polymer (MQ-*g*-PBA). MQ-*g*-PBA was thoroughly investigated for micro-structures by using ^{1}H NMR, ^{13}C NMR, DEPT, 2D NMR (HMBC, HSQC, COSY, NOESY, and TOCSY), and ^{1}H-^{29}Si HMBC NMR spectroscopy. The successful preparation of the graft copolymer was also confirmed by these analyses.

P-3

L-Proline catalyzed multi-component synthesis of N-pyridyl-tetrahydroisoquinolines and their α-C(sp3)-H oxygenation

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Organocatalyzed reactions, using small organic molecules instead of hazardous metal-based catalysts, offer environmentally friendly benefits in synthetic chemistry.[1] Multi-component reactions streamline the creation of complex compounds by combining multiple building blocks in one step, reducing waste and enhancing efficiency.[2] This environmentally friendly and atom-efficient approach accelerates drug development and facilitates materials synthesis in fields like catalysis and materials science. Pyridines are important heterocycles widely used in medicinal chemistry for their water solubility, stability, basicity, and ability to form hydrogen bonds. They find applications in antimicrobial, antiviral, anticancer, and anti-inflammatory treatments.[3] Herein, we report an effective multi-component synthesis that starts with readily available starting materials and accesses poly-substituted pyridine derivatives by using L-proline as a benign catalyst. The process uses cyclic amines, aldehydes, and malononitrile in a condensation reaction to produce a variety of pyridine derivatives under mild conditions. Furthermore, depending on the catalysts used, selective synthesis of amide and/or aldehyde functionality is obtained through α-C(sp^3)-H oxygenation of the tertiary amine moiety in the resultant pyridine derivatives. The pyridine ring's nitrogen atom plays a crucial role in accelerating C-H oxygenation at the α-position of the tertiary amine, highlighting the synthetic versatility and usefulness of this method.

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P-4

Is the Machine-learned mW (ML-mW) model better than the mW Model in representing water's Vapor-liquid Equilibrium?

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Water is crucial for various biological, ecological, industrial, and daily applications. Its extensive hydrogen bonding network imparts unique characteristics, such as high surface tension and elevated melting and boiling points, contributing to over 90 documented anomalies. Due to its complex behavior, more than 100 models have been developed, yet none can fully capture water's properties across all three states-solid, liquid, and gas. Water models generally fall into two categories: all-atom (AA) and coarse-grained (CG) models. While AA models more accurately reproduce water's properties, they are significantly more computationally demanding than CG models. The monatomic mW water model, a popular CG model, is widely used for understanding water's structural, thermodynamic, and solid-liquid coexistence properties and offers a computational efficiency approximately 100 times greater than AA models.[1] However, the mW model does not accurately replicate the vapor-liquid equilibrium (VLE) of water and has a critical temperature that is much higher than expected.[2] Recently, Chan and coworkers[3] developed the ML-mW model by refining the mW model parameters using a multi-level evolutionary machine-learning approach. This new model has been shown to better reproduce water's properties at standard pressure and room temperature. However, its ability to replicate the VLE of water remains unexplored. In this study, we evaluate the accuracy of the ML-mW model in replicating the VLE of water, focusing on properties such as vapor-liquid coexistence densities, surface tension, and critical temperature and pressure (T_c, p_c). Our findings suggest that the ML-mW model performs better than the mW model in reproducing water's VLE. However, it falls short compared to ML-BOP, another CG water model with short-range interactions.[4]

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Targeted Estradiol-Derived Carbon Dots for Selective Induction of Apoptosis in ER (+) Breast Cancer Cells via Oridonin-Activated p53 Pathway

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Breast cancer is one of the most common cancers worldwide, with approximately two-thirds of cases being hormone receptor-positive, particularly involving estrogen receptors (ER). In breast cancers, the tumor suppressor p53, which plays a critical role in regulating cellular functions and preventing tumor growth, is often suppressed. Reactivating p53 can lead to cell cycle arrest and apoptosis, making it a promising strategy for targeted therapy in ER (+) breast cancers.

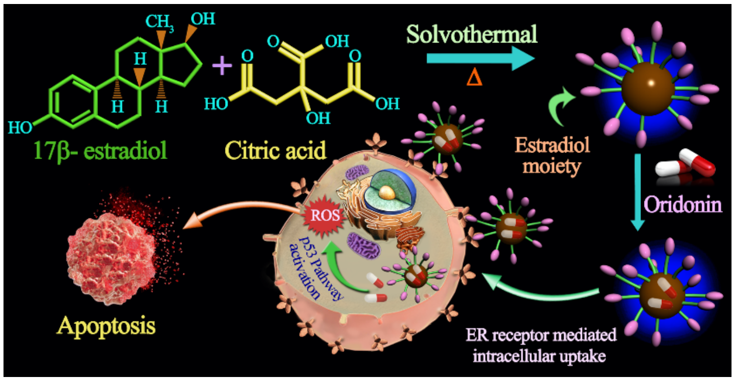

Figure 1. Estradiol-derived carbon dots for selective delivery of oridonin to induce apoptosis in ER (+) MCF-7 cells via upregulation of p53 pathway.

In this study, we designed estradiol-derived carbon dots (**E_2-CA-CD**) using 17*β*-estradiol and citric acid through a solvothermal method. These carbon dots were characterized with various spectroscopic and microscopic techniques. The water-soluble, intrinsically fluorescent **E_2-CA-CD** showed excellent biocompatibility in MCF-7 and MDA-MB-231 breast cancer cells, as well as NIH3T3 normal cells. Importantly, **E_2-CA-CD** enabled targeted bioimaging in ER (+) MCF-7 cells due to their overexpression of estrogen receptors. Oridonin, a well-known hydrophobic anticancer drug that can upregulate the p53 pathway, was loaded onto the carbon dots to enhance the bioavailability (**E_2-CA-CD**-Ori). This formulation exhibited approximately 2.2 times higher cytotoxicity in ER (+) MCF-7 cells compared to ER (-) MDA-MB-231 cells and normal NIH3T3 cells. Furthermore, **E_2-CA-CD**-Ori demonstrated about three times greater efficacy in killing MCF-7 cells than native oridonin. The cell death induced by **E_2-CA-CD**-Ori occurred through an apoptotic pathway, progressing from early to late stages, alongside an increase in intracellular reactive oxygen species (ROS) levels (Figure 1). Notably, **E_2-CA-CD**-Ori activated the p53 pathway in MCF-7 cells, leading to apoptosis through the upregulation of Bax and downregulation of Bcl-2, resulting in selective and effective elimination of ER-positive MCF-7 cells.

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P-6

Gelatin-Statin Microspheres to Modulate Immune Response and Counter Mtb-Induced Immunopathology: A Novel Therapeutic Approach to Target Tuberculosis Pathogenesis

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Tuberculosis (TB) remains a global health challenge, claiming approximately 1.6 million lives annually, making it the second leading cause of death from infectious diseases, following COVID-19 and surpassing HIV/AIDS in mortality. The immune response triggered by *Mycobacterium tuberculosis* (Mtb) is a key factor driving host immunopathology, resulting in excessive inflammation that leads to tissue damage at the site of infection and facilitates transmission to new hosts. This inflammation, mediated by the activation of inflammatory pathways, leads to the degradation of the extracellular matrix (ECM), significantly contributing to the mortality of TB patients [1]. The primary inflammatory mediators, including cytokines such as TNF-α and IL-6, and proteolytic enzymes like gelatinase, are crucial in degrading collagen and other matrix components, further exacerbating tissue damage.

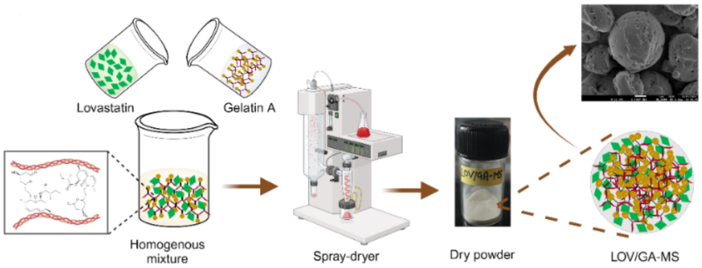

Figure 1. Schematic representation: Synthesis of inhalable LOV/GA microspheres (LOV/GA-MS) using spray-drying.

In this study, we investigated the anti-inflammatory effects of lovastatin, a statin drug, through in vitro experiments. Despite its potential, lovastatin is hindered by poor solubility and low biocompatibility. To address these limitations, we synthesized inhalable gelatin (GA) microspheres using spray-drying technology to enhance the solubility and delivery of lovastatin. The gelatin microsphere effectively increases the bioavailability and solubility of hydrophobic drugs while enabling controlled drug release, making them suitable for pulmonary administration. Their enzyme-responsive characteristics make GA-based systems promising for targeted drug delivery. During infection, gelatinase overexpression in the intracellular environment degrades the gelatin matrix, allowing controlled, "on-demand" release of encapsulated lovastatin at the infected site [2]. The LOV/GA-MS were evaluated for their ability to modulate the immune response in Mtb-infected macrophages. Our results showed a significant reduction in cytokine levels, indicating a strong anti-inflammatory effect. Additionally, we observed a synergistic effect of LOV/GA-MS when combined with conventional anti-TB drugs in vitro, further inhibiting Mtb growth. These findings suggest that inhalable microspheres could serve as a promising "adjunctive therapy" to mitigate the immunopathological damage associated with TB.

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P-7

(Reactivity study of 4-hydroxydithiocoumarin with isocyanide "synthesis of (*E*)-3-((amino)methylene)-2-thioxothiochroman-4-one derivatives" and its cycloadducts)

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Organized by
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In the present protocol, we are trying to focus on the nucleophilic sides of 4-hydroxydithiocoumarin[1,2] by reacting it with Isocyanide, which is also a nucleophile.[3,4] From the consequence of this reaction, we observed that Isocyanide reacts selectivity at the C3 position of 4-hydroxydithiocoumarin to give the product **3,** whereas the other nucleophilic centres, oxygen, and sulphur remain unaffected, hard-hard interaction may be the reason. Both the nucleophile (Isocyanide) and the nucleophile (4-hydroxydithiocoumarin) undergo nucleophilic addition reaction and give rise to the desired product **3a** by forming one C=C bond at the C3 position of 4-hydroxydithiocoumarin. Some of the client feature of the present work are catalyst free, highly atom economy, regioselective, quantitative yield and ambient temperature.

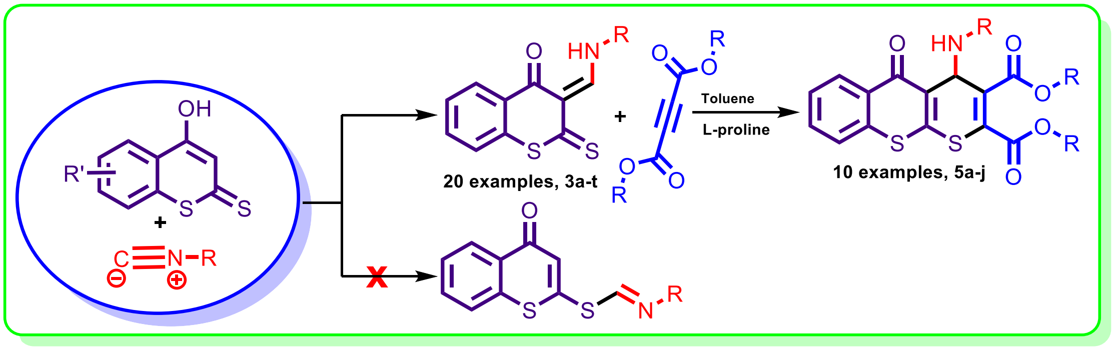

Figure 1.

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Cyclopropenium Salt Catalysed Dimerization of Styrenes

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Catalytic dimerization of aryl alkenes is one of the interesting tools to construct C-C single bond in the organic synthesis.[1] Surprisingly, only a handful of metal catalyzed/mediated protocols have been reported for the dimerization of styrenes.[2] While working on the organocatalytic applications of cyclopropenium salts,[3] we have developed an organocatalytic process for dimerization of styrene using tris(aryl)cyclopropenium salt and the results will be discussed.[4]

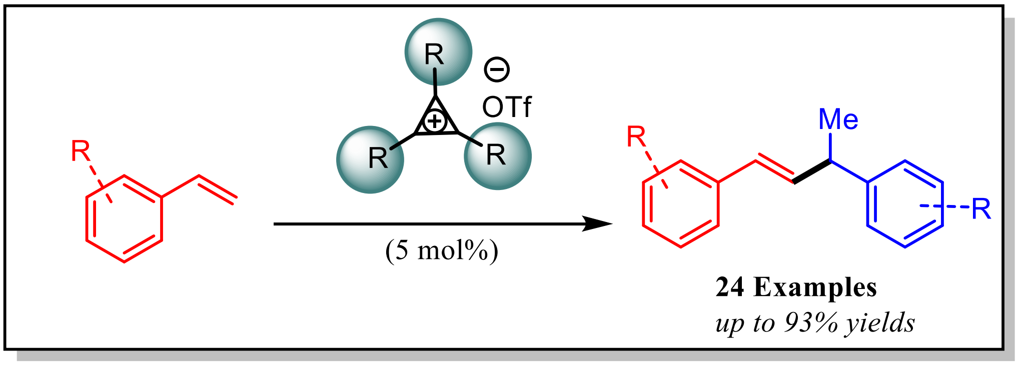

Figure 1. Cyclopropenium ion catalysed Dimerization of substituted styrenes.

Cyclopropenium ions can be effectively used as Lewis acid catalyst to carried out dimerization of styrene to furnish substituted alkenes in good to excellent yield. The reaction proceeds through a cationic mechanism initiated by cyclopropenium ion catalyst to access poly substituted alkenes. Exploring the details of reaction mechanism and the role of triaryl cyclopropenium ions in catalysis are in progress.

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P-9

Chemotactic Directionality of Alkaline Phosphatase in the gradient of carbohydrates and metal ions

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The importance of biomolecular behavior in spatiotemporal control over biological processes and stimuli-responsive nano or micro-machine systems is drawing interest from a wide range of disciplines especially, biomolecular behavior related to taxis in response to chemical gradient at nano- and microscale environment. Since the previous ten years, one of the key areas of discussion in this context is how to understand chemotactic ability and directionality of enzymes in the presence of their substrate gradient. There is mounting evidence that suggests that during the catalytic process, enzyme mobility increases, despite some inconsistent studies that do not agree with this notion.[1] However, the degree of chemotactic drift and directionality are two essential facts that are crucial for the micro- to macroscale prediction and design of biochemical spatiotemporal response patterns. Most of the time, enzymes including urease, catalase, acetylcholine esterase, kinase, phosphatase, DNA polymerase, and many more are known to have the ability to chemotactically move in response to a gradient of their substrate in a microfluidic environment.

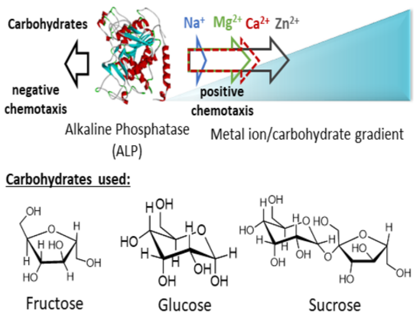

Figure 1. Schematic representation of the extent and directionality of chemotactic drift in response to the gradient of salts and carbohydrates.

Thus, new questions are posed: what will be the taxis behavior for only enzymes with respect to physiologically relevant ions or carbohydrates in a solely non-catalytic environment. Notably, there are few studies addressing how interactive or non-interactive ions or molecules affect an enzyme's chemotactic directionality when it is not catalysing. Herein, we report the extent and directionality of the chemotactic property of the membrane-bound glycoprotein alkaline phosphatase (ALP), a physiologically and clinically significant enzyme, in relation to a gradient of metal ions (Na^+, Ca^{2+}), including its metal ion co-factors (Mg^{2+} & Zn^{2+}) and carbohydrates osmolytes (glucose, fructose and sucrose). It was observed that ALP migrates slightly away from the gradient of carbohydrates, while the direction of migration for divalent metal ions is opposite and more pronounced. This differential phoresis is due to Hofmeister effect driven change in ALP surface zeta potential and osmotic pressure imbalance.[2] The ability to regulate an enzyme's chemotactic extent and direction in response to entirely non-catalytic conditions may prove useful in the fabrication of environment-responsive and biomedical nanomachines. Also, Plasma based micropump will be shown where manipulation of acetylcholinesterase's (present in human plasma) activity has been performed in presence of acetylcholine (a neurotransmitter) and different nucleotides.[3]

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P-10

Interplay of Capacitive and Diffusion Contributions in Redox Active Complex Metal Oxide Rods Channelled into MXene For Improved Charge Transfer Dynamics

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A synergistic approach combining capacitive and redox-active materials is employed to develop supercapacitors that effectively bridge the gap between traditional supercapacitors and batteries in terms of their high-power delivery and increased energy storage capacity. Here we have reported MXene with manganese vanadium oxide ($Mn_2V_2O_7$) nanorods to eliminate the limitations such as restacking of MXenes, which poses a major problem in achieving high conductivity to be used in supercapacitor applications. Formation of pathways for ion migration in $Mn_2V_2O_7$/MXene composite resulting in increased conductivity, enhanced ion transport capacity, and structural stability in aqueous electrolytes, leading to superior performance with a specific capacitance of 627 F g^{-1} at 1 A g^{-1}. Assembled device $Mn_2V_2O_7$/MXene//AC gives a high potential window of 2 V with a high specific energy of 64.1 Wh kg^{-1} at a power density of 1000 W kg^{-1}. Additionally, complex impedance spectra analysed via Distribution of Relaxation Time (DRT) offer enhanced insights into charge transfer kinetics.[1,2]

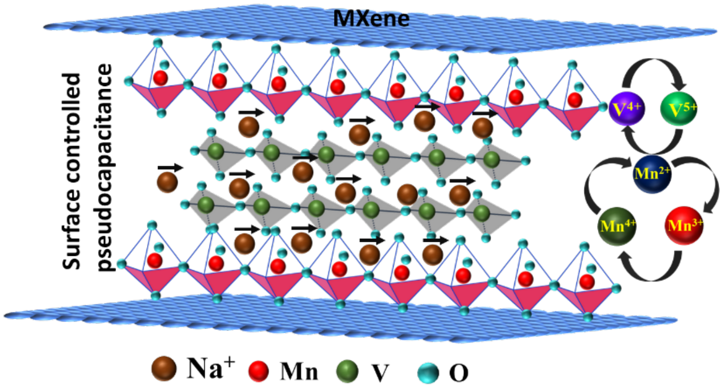

Figure 1: Probable Mechanism of charge storage in $Mn_2V_2O_7$/MXene composite

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P-11

Photocatalyst-Free N-Arylation of Secondary Amines Under Visible-light Irradiation

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A straightforward and useful technique for N-arylation of numerous sets of secondary amides/amines has been achieved via visible light irradiation. It is effective approach for its photocatalyst-free and more environmentally friendly methodology, in which different type of secondary amines were arylated via electron donor-acceptor (EDA) complex. This complex provides a novel pathway for the synthesis of compounds with pharmacological importance and acts as an intermediate for the formation of desired products. This methodology has a number of benefits, including better yields, greener energy consumption, and milder reaction conditions.

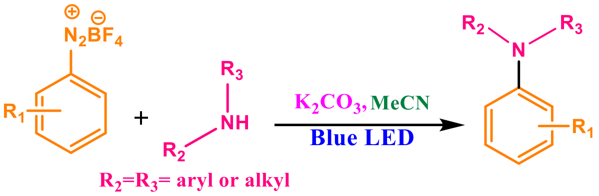

Figure 1. N-arylation of secondary amines

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P-12

Organotin (IV) derivatives with 2-hydroxy-5-((4-(trifluoromethyl)phenyl)diazenyl)benzoic acid: Synthesis and structures

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In the recent times, there has been an increasing interest in the molecular architectures involving organotin (IV) carboxylates. Self assembly of organotin (IV) carboxylate is particularly attractive since it can be accomplished in one-pot reactions and allows for easy fine-tuning of structural and functional features [1]. The construction of multi-dimensional architectures depends mainly on the combination of several factors including the type of organic ligands, tin-R groups, tin coordination geometry preferences and tin-to-ligand molar ratio. In addition, the hydrogen bonding interaction also play key roles in the generation of a variety of molecular structures [2].

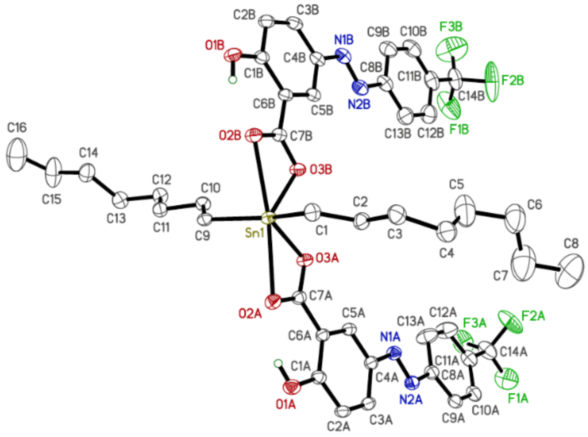

Figure. 1. Ellipsoid plot of n-Oct$_2$Sn(L)$_2$ (**3**) with atom labeling scheme.

In this context, some organotin(IV) complexes of compositions *viz*., R$_2$Sn(L)$_2$: (R = Me (**1**), n-Bu (**2**), n-Oct (**3**), Figure. 1) and R$_3$SnL: (R = n-Bu (**4**) and Ph (**5**)) were investigated. The synthetic details, spectroscopic characterization and structural aspects will be presented.

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P-13

Highly Efficient Main-Chain Cationic Polyelectrolytes for Selective and Sensitive Detection of Biomolecules Heparin and Toxic Oxoanions Perrhenate and Permanganate

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Development of new chemosensors with high sensitivity and selectivity is very essential for the detection of biomolecules (anti-coagulant like heparin) or toxic oxoanions (TcO_4^-, MnO_4^-). Pertechnetate is a radioactive oxoanion, which are produced during radioactive research, power generation, and fuel-rod processing. Due to its remarkable long half-life ($t_{1/2} = 2.13\times10^5$ years), high solubility in water, and exceptional kinetic stability, it increases the risk of water pollution and poses a threat to the human health and aquatic ecosystem.[1] However, the restriction in handling this radioactive element constraint their detection. During surgery and post-operative phase, heparin level monitoring and quantification is essential to prevent any undesirable circumstances including osteoporosis, haemorrhage, and thrombocytopenia due to over-dose.[2] However, the conventional techniques for heparin detection are expensive, time-consuming and suffers from poor selectivity due to the interference from other biological molecules.

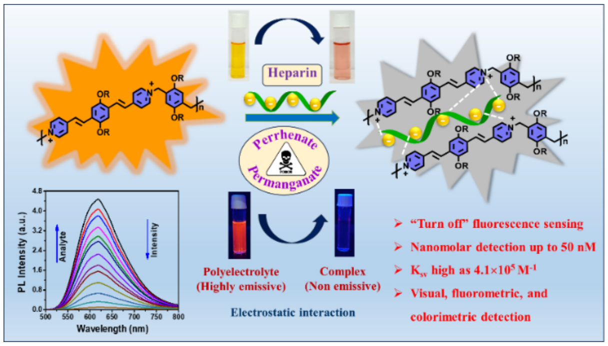

Figure 1. Main-chain cationic polyelectrolytes for selective and sensitive detection of multiple analytes in nanomolar scale by aggregation or complexation induced emission quenching.

Here, we have synthesized a set of *p*-phenylenevinylene unit containing cationic main-chain polyelectrolytes with various alkoxy side-chains by substitution polymerization, which exhibited vivid orange fluorescence and functioned as "turn off" fluorescent probes for selective detection of hazardous inorganic oxoanions perrhenate and permanganate as well as essential biomolecule heparin.[3] For heparin, a very low detectability of 50 nM was observed with a high Stern-Volmer constant (K_{sv}) of 4.1×10^5 M^{-1}. Also, they demonstrated selective sensing of MnO_4^- (LOD = 20×10^{-8} M and $K_{sv} = 5.6\times10^4$ M^{-1}) and ReO_4^- (LOD = 5.8×10^{-7} M and $K_{sv} = 45\times10^3$ M^{-1}) among other inorganic anions. Absorption spectra revealed that, in the case of heparin and perrhenate, sensing was presumably due to aggregation-caused quenching, whereas MnO_4^- ions were detected through interactions with the vinylic unit of polyelectrolyte. Our polyelectrolytes are effective multifunctional materials with capability of detecting essential biomolecules as well as toxic oxoanions using both colorimetric and fluorometric methods, which offer promising methodology for real-time monitoring purpose.

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P-14

Photophysical and computational studies on an HSA selective D-π-A probe

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Human serum albumin is an essential indicator of the health status of any individual.[1] Hence, its accurate estimation can be used for disease prediction and diagnosis.[2] To cater to this need, we have developed a series of donor-π-acceptor probes for the selective detection of HSA. Among the probes developed, the trifluoroacetyl group-bearing probe A4 was the most sensitive, with the detection limit being 1.36nM.

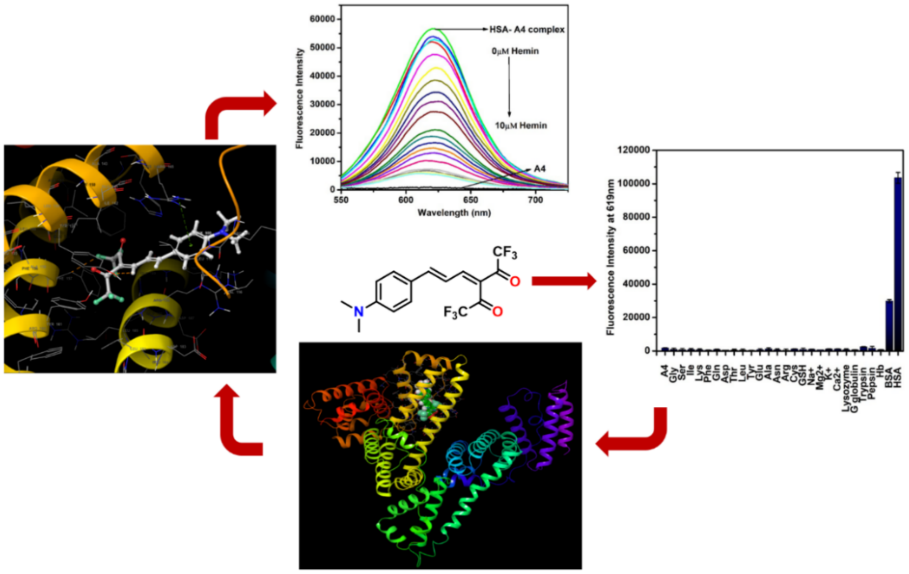

Figure 1. Human serum albumin HSA conjugate.sensing using probe A4 and hemin sensing using A4-

The probe works on the principle of excited state intramolecular charge transfer. The fluorescence displacement assay revealed the probe's localization at its hemin binding site IB, which was further validated using molecular docking and MD Simulations. Computational experiments shed light on the change in preference of A4 towards HSA amino acids Tyr161, Met123, Pro118, and Leu115 in the excited state when compared to that observed in the ground state (Arg186 and His146). It was observed that ground-state interactions involved water bridges in addition to hydrophobic interactions, whereas excited-state interactions were purely hydrophobic. The utility of probe A4 was explored in sensing HSA in urine at extremely low concentrations. The A4-HSA conjugate was also used as a hemin sensor and exhibited a detection limit of 0.23μM.

Details of the work done will be presented during the oral presentation.

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P-15

Site-specific incorporation of a synthesized triazolyl unnatural amino acid, using genetic code expansion into T7-RNA-polymerase in vivo.

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T7 RNA polymerase is a widely utilised enzyme in molecular biology research due to its excellent specificity and efficiency in transcribing RNA from DNA templates.[1] T7 RNA polymerase mutations can alter substrate binding, catalytic activity, or fidelity of RNA synthesis by interfering with vital interactions within the active site of the enzyme. One such hotspot is the Y571 site which plays a crucial role in its catalytic activity and promoter recognition. Because of its close proximity to the active site, the 571st codon position in T7 RNA polymerase is crucial for regulating both the overall catalytic efficiency and the interactions between the enzyme and substrate. Being a mutation hotspot, the Y571 is prone to being mutated into a serine residue, due to a point mutation in the codon of tyrosine from UAC to UCC. The catalytic activity and substrate recognition of T7 RNA polymerase are significantly altered when the codon for tyrosine 571 (Y571) is mutated to serine.[2,3]

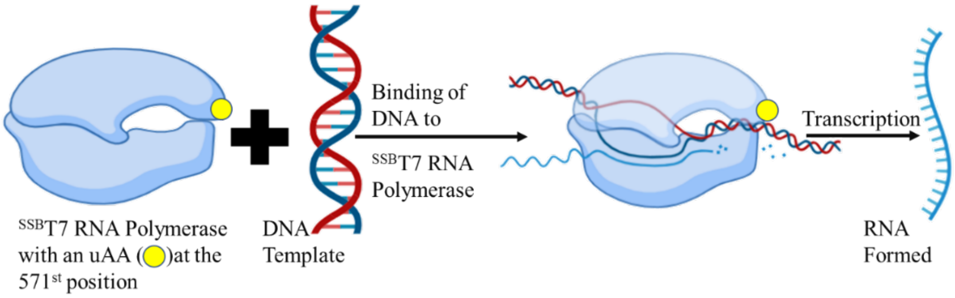

Figure 1. Graphical abstract depicting the transcription mechanism of DNA to RNA using **^{SSB}T7 RNA Polymerase**

Therefore, this study demonstrates the novel creation of an improved T7 RNA polymerase enzyme containing a structural analogue of tyrosine, a fluorescent triazolyl unnatural amino acid (FTUAA)[4,5] incorporated at codon position 571. With this accomplishment, the genetic code expansion[6] approach succeeded in incorporating a triazolyl amino acid into a protein for the first time. We have also recorded that the modification at this codon site can dramatically change the characteristics of the enzyme and provide a mechanism for tailoring its activity for specific uses. The genetic code expansion strategy is pivotal for this work as it allows the incorporation of various non-canonical amino acids into proteins. Towards this end, the triazolyl group, introduced via the unnatural amino acid, offers unique benefits due to its stability, rigidity, ability to engage in diverse chemical interactions and enhanced photophysical properties. Overall, our research demonstrates the feasibility and potential of incorporating unnatural amino acids into key positions of enzymes to engineer novel functionalities, paving the way for advanced applications in various scientific and industrial fields.

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P-16

CO_2 Photoreduction integrated with oxidative coupling of amines over WO_3/Cu(BTC) nanocomposite

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Here, we developed an efficient integrated CO_2 photoreduction to methanol accompanied with the simultaneous oxidation of benzyl amines to corresponding imines using quadrangular WO_3 nanoplates grafted with Cu(BTC) as a photocatalyst under visible light, enabling to provide efficient use of the photogenerated electrons and holes. Under the optimized reaction conditions, the maximum yield of methanol and *N*-(4-methoxybenzyl)-1-(4-methoxyphenyl)methanimine was found to be 642 μmol-g^{-1} and 98%, respectively. The developed integrated dual functional system comprising CO_2 reduction coupled with the oxidative organic synthesis opens a new window for value chain upgradation at both ends using sustainable solar energy.

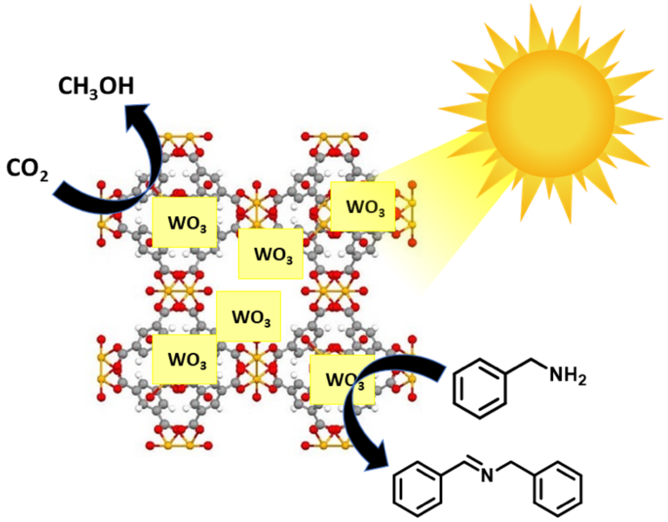

Figure 1. Graphical abstract of photoreduction of CO_2 to methanol accompanied with the simultaneous oxidative coupling of amine to imine.

P-17

Surfactant-Induced Alterations in Optoelectronic Properties of Perylene Diimide Dyes: Modulating Sensing Responses in the Aqueous Environment

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The compartmentalization effect in microheterogeneous systems, such as surfactant aggregates, enhances the sensitivity of polyaromatic dye molecules toward target analytes by impeding their aggregation in aqueous media. The micellar environment features reduced hydration, low micropolarity, and high local concentrations of dye molecules, which significantly alter their acid-base properties compared to bulk water. Additionally, restricted water dynamics at the micelle-water interface improve non-covalent interactions (e.g., hydrogen bonding, charge pairing) with analytes. While most sensors are designed for detecting ionic analytes or biomolecules in bulk media, few studies have explored optical sensing in membrane-bound states. Detecting interfacially bound analytes is crucial for understanding cellular transport pathways and mechanisms of toxicity.

Given that local environmental changes affect the excited-state properties of dye molecules—such as fluorescence quantum yield, lifetime, and spectral characteristics—we investigated whether micellization influences their sensing properties. We synthesized a perylene diimide-based chromogenic dye with alanine residues (PDI-Ala), selected for its exceptional optoelectronic properties, including high fluorescence quantum yield, photostability, and narrow emission bands. This chemical stability ensures long-term functionality, even in harsh conditions. The tunable emission properties and compatibility with various substrates allow for customization, enabling advancements in environmental monitoring, biomedical diagnostics, and food safety.

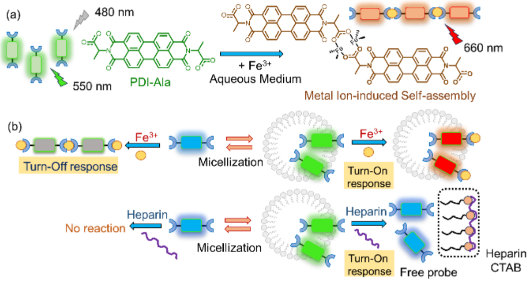

Figure 1. (a) Schematic diagram shows the formation of metallo-supramolecular assembly of PDI-Ala in the presence of Fe^{3+}. (b) Schematic diagram shows changes in sensing response of PDI-Ala in the presence of surfactant aggregates.

The compartmentalization effect in microheterogeneous systems, like surfactant aggregates, alters the optoelectronic properties of a perylene diimide-based chromogenic dye (PDI-Ala) compared to bulk water. The hydrophobic microenvironment, poor hydration, and high local concentration of dye molecules influence their interactions with target analytes. This led us to investigate how micellization affects the sensing properties—such as selectivity, sensitivity, response kinetics, and output signal—of encapsulated dye molecules in aqueous media. Comparing the responses of PDI-Ala to ionic analyte (Fe^{3+}) and biomolecule (heparin) in aqueous versus surfactant-bound states revealed significant variations. In water, Fe^{3+} produced a "turn-off" fluorescence response, while in the surfactant-bound state, it triggered a "turn-on" response, enhancing selectivity at the micelle-water interface. Conversely, the native probe showed no interaction with heparin in water but displayed a turn-on fluorescence response in Cetrimonium bromide (CTAB) micelles, effectively transforming a silent molecule into an active fluorescence sensor. This study highlights how micellar environments can alter the sensing responses and selectivity of dye molecules, which is crucial for applications in understanding cellular pathways and mechanisms of toxicity.

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P-18

Synthesis and characterization of a new five-coordinated, one-dimensional coordination polymer of cobalt (II) with 2,2'-([1,1'-biphenyl]-2,2'-diylbis(oxy))diacetic acid.

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Synthesis and characterization of a new five-coordinated, binuclear one-dimensional coordination polymer of cobalt (II) with 2,2'-([1,1'-biphenyl]-2,2'-diylbis(oxy))diacetic acid are described. It involves reaction of 2,2'-([1,1'-biphenyl]-2,2'-diylbis(oxy))diacetic acid and cobalt nitrate hexahydrate in DMF and to increase structural variation of the complex 4,4'-bipyridyl has been added as an ancillary ligand. Even though five-coordinated cobalt complexes are very rare, but have some complexes [1-4]. Cobalt (II) complexes shows different g-values pattern as a consequence of geometrical distortions and of variations in the ligand field strength in the ESR spectra[2]. In this complex cobalt (II) has five-coordination number with distorted trigonal bipyramidal geometry having triclinic crytal structure and P-1 space group. The structure of the new complex has been characterized by FTIR and single X-ray Crystallography technique. The self assembly and stability of the crystal structure are supported by intermolecular H-bond between the polymeric chain and also by other weak interactions like C-H$\cdots$O, C-H$\cdots\pi$ and $\pi\cdots\pi$ etc.The crystal structure of the complex is shown in **fig.1**

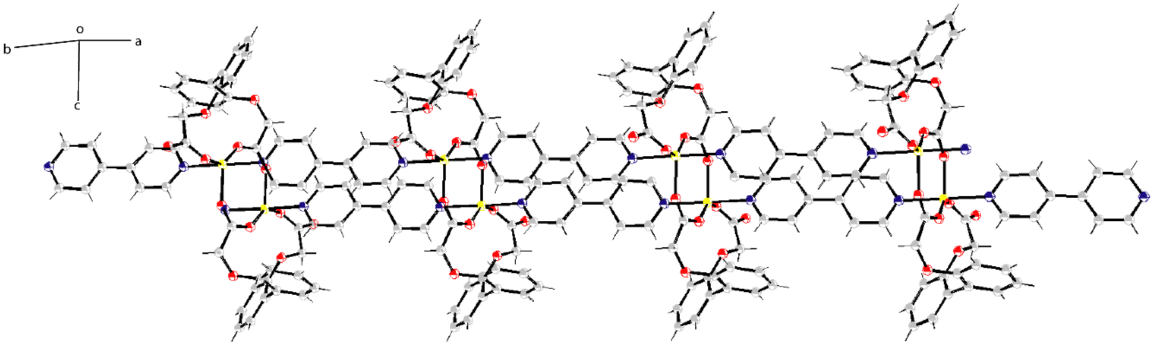

Fig 1: Self-assembly of five-coordinated, binuclear one-dimensional coordination polymer of cobalt (II) complex with 2,2'-([1,1'-biphenyl]-2,2'-diylbis(oxy))diacetic acid

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P-19

Synthesis and Characterization of Co-Mn-MoS_2 Composites for Improved Hydrogen Evolution Reaction Performance

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Hydrogen Evolution Reaction (HER) is a key process in electrochemical water splitting, crucial for sustainable hydrogen production. Developing efficient, low-cost catalysts is essential to improving HER efficiency. Transition metal sulfides, particularly molybdenum disulfide (MoS_2)-based composites, have gained significant attention due to their promising catalytic properties. In this work, we focused on the hydrothermal synthesis of cobalt-manganese-MoS_2 ternary composites, and explored its potential towards HER activity.

The sample was synthesized using cobalt nitrate, potassium permanganate, and sodium molybdate as precursors, along with L-cysteine as a sulfur source, using low-temperature hydrothermal technique. X-ray diffraction confirmed the phase formation of Co-Mn-MoS_2 with characteristic peaks, while field-emission scanning electron microscopy revealed the formation of clustered nanostructures with Co and Mn doping leading to surface roughness, which increased the active sites for HER. Energy-dispersive X-ray spectroscopy provided the stoichiometric information of the sample. Electrochemical measurements showed that the Co-Mn-MoS_2 composite exhibited good HER performance, with low onset potential and small Tafel slope compared to pure MoS_2.

These findings demonstrate the potential of the as-synthesized ternary hybrid as a promising electrocatalyst for efficient hydrogen production and contribute effectively in the field of sustainable energy.

Keywords: HER, MoS_2, Composites, Electrocatalyst, Overpotential

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P-20

"Eco-Friendly Synthesis and Characterization of Bimetallic Nanoparticles"

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Nanotechnology has been a controversial topic for the past few decades, but new advancements have made it much more interesting. Because of their widespread use in a variety of technological applications, nanoparticles are "tiny heroes" that carry out tasks that would otherwise be impossible. Natural extracts facilitate the production of BNPs in an easy, cheap, and environmentally friendly approach. Phenolic substances contained in plant extract function as stabilizing ligand moieties (carbonyl, carboxyl, and amine groups) and reducing agents (flavonoids, terpenoids, tannins, and alkaloids). These compounds are also free of hazardous byproducts and can be used in the environmentally friendly creation of nanoparticles (NPs). The current study focuses on use of Azadirachta Indica leaf extracts to create iron-nickel bimetallic nanoparticles.The synthesized nanoparticles were characterized by spectra of a UV–vis spectrophotometer during the synthesis process. The maximum absorption wavelength at 268 nm was observed, confirming the formation of bimetallic nanoparticles. Fourier transform infrared spectroscopy (FTIR) studies showed that the plant extract's C=O and C-O groups were crucial for capping the nanoparticles. Importantly, the process can be called pure "green chemistry" since no additional synthetic chemicals are required for the purpose of stabilization or reductant. More intriguing than metal nanoparticles are bimetallic nanoparticles, which are composed of two metal nanoparticles that combine in an uncommon way and have a synergistic effect. Thus, the disciplines of agriculture, medicine, and environmental cleanup will employ the produced nanoparticles.

Key words: Nanotechnology;Green synthesis;Azadirachta indica; Bimetallic nanoparticles.

P-21

Bioactive Polyphenols and Their Antidiabetic Potential and Inhibitory Effects on Starch Digestive Enzymes: A Novel Approach for Diabetes Management

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With the current global surge in occurrence of diabetes, studies focus on procurement of natural products for diabetes management. Current medications of diabetes have adverse negative side effects for patients and to minimize these, natural bioactive compounds are investigated for their effect on diabetes management. Polyphenols are a diverse group of naturally occurring compounds found in plants which have garnered significant attention for their potential effects on blood glucose regulation. Polyphenols consist of several groups of chemical compounds such as phenolic acids – ex. tannic acid, gallic acid; flavonoids ex.- flavonols, flavonones; stilbenes and polymeric lignans. They can be extracted from different plant source and also available in plenty of amount in our daily diet.

This study examines the impact of dietary polyphenols on glucose metabolism, highlighting their role in insulin sensitivity, carbohydrate digestion, glucose absorption, and the modulation of gut microbiota. Numerous studies suggest that polyphenols, mainly flavonoids and phenolic acids, can enhance insulin action and reduce postprandial glucose levels. Mechanistically, polyphenols may influence pathways related to oxidative stress, inflammation, and enzymatic activity involved in carbohydrate digestion. This study also explores mathematical simulation of starch digestion under *in vivo* conditions and further estimates the rate of glucose formation in MATLAB. Polyphenols such as tannic acid and gallic acid have shown inhibitory effects on the key enzymes for starch digestion i.e, α-amylase and α-glucosidase, thus modulating the starch hydrolysis and affecting the postprandial glucose levels. Using mathematical models on Rate Law kinetics and Michaelis-Menten equations for enzyme kinetics, we have performed preliminary studies on the rate kinetics of the formation of these metabolites and the inhibition of the enzymes by the polyphenols. The results of the kinetic assay are graphically represented using MATLAB simulation and interpreted which shows that polyphenols when in higher concentration act as competitive inhibitors for the amylase, glucosidases and intestinal brush border enzymes. Polyphenols also have effect on glucose transporters across the epithelial membranes thus also slowing down the glucose absorption rate, thus reducing postprandial hyperglycemic spike.

Furthermore, the interaction between polyphenols and gut microbiota appears to enhance their bioavailability and efficacy. While results are promising, the variability in individual responses and the complexity of polyphenol interactions necessitate further research to establish specific dietary recommendations and therapeutic applications. Overall, polyphenols represent a promising avenue for managing blood glucose levels, particularly in the context of metabolic disorders such as type 2 diabetes.

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P-22

Vanadium doped cobalt selenide: a potent oxygen evolution electrocatalyst

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An economical and effective electrocatalyst is the need of the hour to overcome the sluggish oxygen evolution process to be used in practical applications for rechargeable energy storage technologies and water splitting for the production of clean fuel. So, in this work, we have synthesized a series of vanadium-doped cobalt selenide ($Co_{0.75}V_{0.25}Se_2$, $Co_{0.5}V_{0.5}Se_2$, $Co_{0.25}V_{0.75}Se_2$) by varying the concentration of Co and V. Among the synthesized materials, $Co_{0.75}V_{0.25}Se_2$ has exhibited excellent performance towards the Oxygen Evolution Reaction (OER). $Co_{0.75}V_{0.25}Se_2$ facilitates the sluggish kinetics of the OER mechanism and leads to a low overpotential value of 315 mV at the current density of 10 mA/cm^2 and has a lower Tafel slope of 63 mV/dec. The efficiency of the electrocatalyst can be attributed to the V doping, which led to an enhancement in the number of electroactive sites for the process of OER. The electrocatalyst shows 16 hr stability at 10 mA/cm^2 current density, enhancing its practical durability as an effective catalyst for anodic OER in the water electrolysis process.

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P-23

Enhancing the flame retardancy of natural leather using carbonate-based inorganic salt: synthesis, characterisation, and application studies

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Flame Retardants are added to various consumer products during manufacturing to prevent or slow down the further spread of fire. But, most of the flame retardants available on the market are toxic to the environment or humans. Hence sustainable development is needed in the field of flame retardants. Leather is a natural by-product of the food industry, almost seven million tonnes would go to landfills if not utilized appropriately. Also, leathers are long-lasting, repairable, and recyclable; hence it is a sustainable contribution to society. Leather has varied end uses and some special application requires flame retardant properties. The objective of this research work; is to develop an environment-friendly and nontoxic flame retardant for leather application. As per the literature reports, carbonates are potential flame retardant (FR), since they can undergo endothermic thermal degradation.[1] Also, the carbon dioxide evolved during the thermal degradation of carbonates; dilutes the combustible gases, and lowers the partial pressure of oxygen around the flame.[2] Magnesium carbonate (MC) was chosen as a promising flame retardant for leather, because they are non-toxic, environment-friendly, a carbon sequestration agent, and cost-efficient.

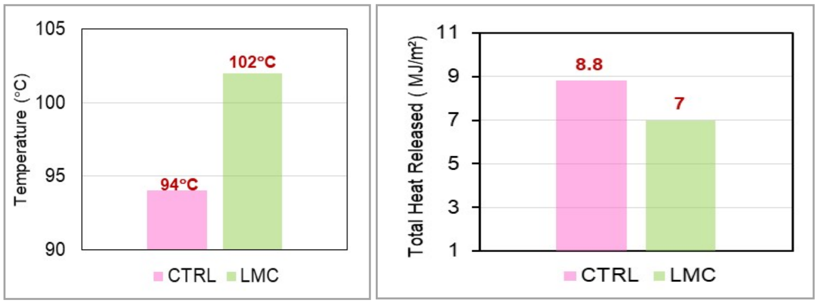

Figure 1. a) Shrinkage temperature and b) Total Heat Release of the control (CTRL) and MC treated (LMC) leathers

Six different magnesium carbonates were synthesised by varying the precursor salts and synthesis methods. The synthesised and commercial MC were characterised using XRD, FTIR, DSC, particle size, and zeta potential. The DSC thermogram revealed high endothermic heat change indicating that MC can be a potential flame retardant. The synthesised and commercial MC was applied to natural leather during the post-tanning stage of conventional leather processing. The control leather (CTRL) is processed by following the same process but without adding MC. The flame retardancy properties of the MC-treated leathers were studied for shrinkage temperature by shrinkage test (SATRA TM 17:1997), flammability degree by horizontal flame retardancy test (ISO 17074), and a whole set of parameters like sample mass loss (SML), total heat released (THR), peak rate of heat release (PRHR), average RHR (ARHR), and average effective heat of combustion (AEHC) using cone calorimeter test (ISO 5660).[3] Figure 1 shows that the shrinkage temperature was improved by 8°C (Fig. 1a), and THR was improved by 20% (Fig. 1b) for the MC-treated leather compared to the control leather. An effort was made to understand, the correlation between the morphology and particle size of the synthesized MC to the flame retardancy of MC-treated leather.

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P-24

Process development for the total synthesis of the novel drug metabolite Carboxy toremifene as a standard reference material along with characterization and purity assessment for the Antidoping quality Control Purposes

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Tamoxifen and toremifene are two selective estrogen receptor modulators (SERMs) commonly used to treat breast cancer in women.[1] Toremifene is well-known as a triphenylethylene derivative. Carboxy toremifene is a common metabolite of toremifene and tamoxifen.[2] Since 2005, the World Anti-Doping Agency (WADA) has banned the SERMs category during in and out of competition.[3] These substances are in the S4 category in the WADA prohibited list as "agents with anti-oestrogenic activity." [4] However, there is no commercially accessible carboxy toremifene reference material in the market. This research highlights the novel synthetic procedure, the development of a carboxy toremifene HPLC method, and validation, along with detailed characterization using advanced analytical techniques using ^{1}H NMR, HRMS, FT-IR-ATR and UV–visible spectroscopy. RP-HPLC-DAD method was developed and validated to assess the purity of carboxy toremifene.[5] Developed reference material has shown 100% purity. Therefore, we recommend that this synthesized carboxy toremifene may be used as reference material to strengthen the WADA-accredited lab to maintain a clean sports mission during sports competitions.

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P-25

An efficient biocatalysed synthesis of 2-aryl chromones through oxidative cyclization

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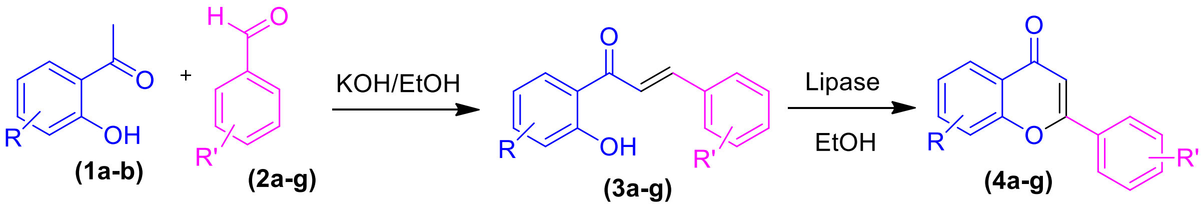
Keywords CAL-B lipase, oxidative cyclization, 2-aryl chromones.

Biocatalysis is the process of acceleration of the rates of specified chemical transformations using biocatalysts. Rapid access to enzymes with a variety of natural and even unnatural catalytic activities has expanded the synthetic organic chemist's toolbox. A convenient and efficient oxidative cyclization of 1-(2'-hydroxyl phenyl)-3-aryl-2-propen-1-ones, accelerated by lipase, CAL-B has been first time carried at room temperature and obtained 2-aryl chromones with better to excellent yields. The developed protocol has simplicity, eco-friendliness and cost-effectiveness. The details of the optimization and advantages of the protocol than those already practiced will be debated.



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P-26

Ruthenium (II)-catalyzed C-H activation/annulation of pyrroline carboxylates with alkynes: synthesis of 2,3-diphenylspiro-[indene-1,2′pyrrolidine] carboxylate derivatives

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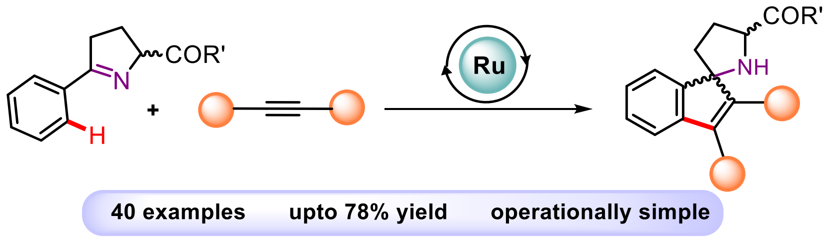
Saturated nitrogen heterocycles are essential frameworks found in both natural products and pharmaceutical compounds.[1] They account for 5 out of top 10 ring structures in pharmaceuticals.[1a] Among these pyrrolidine ring is present in different bioactive natural products and pharmaceuticals and subsequently they are highly valued as essential building blocks in medicinal chemistry and as candidates in fragment-based drug discovery.[2] The pyrrolidine ring is especially important as a constituent of the cyclic amino acid proline, frequently employed by nature to facilitate various secondary structures in proteins[3a] and as effective catalysts for achieving stereoselective synthesis.[3b] Hence, the synthesis of substituted proline derivatives is highly desirable.



40 examples upto 78% yield operationally simple

Figure 1. Ru (II) catalyzed C-H activation/annulation of pyrroline carboxylates with alkyne

While saturated nitrogen heterocycles are privileged scaffolds, their streamlined catalytic synthesis with unsymmetrical substitution patterns remains a daunting challenge. We first report ruthenium (II) catalysed synthesis of spiro-[indene-proline] derivatives via C-H activation/annulation of pyrroline carboxylates with alkynes. The protocol utilized imine coordination, resulting in high reaction yields with a wide range of functional group tolerance, scalability, and scaffold diversity. This annulation was successful even with various biologically active pharmacophore scaffolds. The reaction featured a reversible C–H metalation step and suggested the possibility of a base-assisted internal electrophilic substitution pathway.

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P-27

Highly selective solution and film based sensor for colorimetric sensing of arginine in aqueous and blood samples.

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Arginine is a vital amino acid involved in various physiological processes, including nitric oxide synthesis and immune response [1]. Alterations in arginine levels have been linked to several health conditions such as cardiovascular diseases, metabolic disorders, and immune dysfunctions [2]. Accurate and sensitive detection of arginine in biological fluids like blood is critical for early diagnosis and monitoring of these conditions. Traditional methods for arginine detection involve complex analytical techniques which are often time-consuming and expensive. Therefore, developing a simple, cost-effective colorimetric sensor could be a valuable tool for rapid arginine detection in clinical and diagnostic settings.

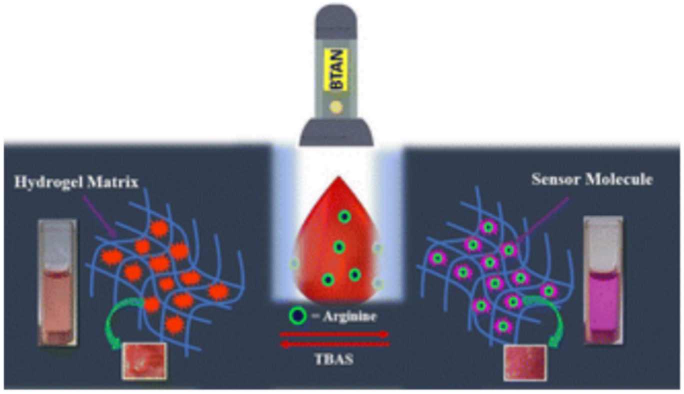

Figure 1. Graphical representation of arginine sensing by BTAN

We have designed and synthesized a benzothiazole-azo based optical sensor BTAN for arginine among other 12 naturally available amino acids in semi aqueous media i.e. DMSO-H_2O (1:1, v/v) [3]. It was quite fascinating to see the rapid colour change from orange to pink on addition of arginine within 2-3 seconds which was easily discernible by naked eye. The detection limit for arginine was as low as 0.7 µM. The sensor's detection process, studied using 1H-NMR and UV-vis spectroscopy, based on deprotonating the -OH group of BTAN when it interacts with arginine, causing a visible colour change. For practical use, BTAN was immobilized into a starch-PVA hydrogel and paper strips, allowing effective on-site detection in fully aqueous environments. The sensor also showed excellent ability to avoid interference from other amino acids, which is uncommon in amino acid sensors. Additionally, the sensor was successfully tested for detecting arginine in human blood samples, offering a fast, easy, and versatile method for both qualitative and quantitative arginine detection.

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P-28

Synthesis of Highly π-Extended Dihydrobenzo[*a*]indenocarbazole Scaffolds via Tandem Benzannulation and Friedel–Crafts Reaction of 2-Alkynylanilines and 2-Alkynylbenzaldehydes Promoted by Lewis Acid

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A novel and efficient tandem protocol for the swift synthesis of dihydrobenzo[*a*]indenocarbazole frameworks from 2-alkynylanilines and 2-alkynylbenzaldehydes via $BF_3 \cdot OEt_2$-facilitated benzannulation and Friedel–Crafts reaction has been described. This innovative approach accommodates a wide array of functional groups, offering a myriad of diversified carbazole products. Later, postsynthetic modification leads to its C(sp^3)-H hydroxylation. Furthermore, the photophysical properties of some selected synthesized moieties have been meticulously investigated, promising exciting avenues for further exploration.

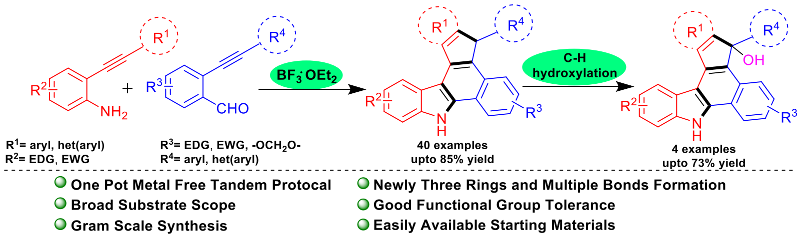

Figure 1. Graphical abstract of the synthesis of dihydrobenzo[*a*]indenocarbazole and its derivatives

Carbazoles are privileged tricyclic nitrogen-containing heterocyclic motifs with the carbon skeleton of fluorene, ubiquitous in numerous alkaloid-based natural products, pharmaceutically relevant compounds, and functional materials. They have garnered significant attention in the monarchy of organic chemistry due to their versatile applications and intriguing properties. With a distinctive structure composed of two benzene rings fused to a pyrrole ring, carbazole exhibits remarkable stability and reactivity, making it a cornerstone in the synthesis of various organic compounds. Its conjugated system and electron-rich nature make it a prime candidate for optoelectronic materials, including organic light-emitting diodes (OLEDs), photovoltaics, and sensors. Moreover, carbazole derivatives have demonstrated notable biological activities, ranging from anticancer and antimicrobial properties to enzyme inhibition. This multifaceted compound continues to captivate researchers worldwide, driving advancements in both fundamental studies and practical applications. Within the large varieties of carbazoles, benzo[*a*]carbazoles are an important class of this family, and have received much attention in medicinal chemistry and fine chemical industry owing to their promising biological activities and unique thermal stability properties. Expanding on previous breakthroughs along with various metal-mediated and multistep strategies, our metal-free tandem protocol innovatively forms one C–N bond and three C–C bonds. Utilizing only a Lewis acid, it efficiently constructs highly π-extended benzo[*a*]carbazole scaffolds, marking a significant advancement in synthesis techniques.

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P-29

Nitrogen, sulfur codoped MXene quantum dot – a superior HER electrocatalyst

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MXenes, which are transition metal carbides/nitrides or carbonitrides have very good electrochemical properties and focused as a promising candidate as an electrocatalyst for several reactions such as hydrogen evolution reaction (HER), oxygen evolution reaction (OER) etc [1]. However, the electrocatalytic performance of two-dimensional (2D) MXenes is significantly constrained by the lack of number of active sites in the basal plane. This problem can be solved significantly by reducing the size of 2D MXene into zero-dimensional (0D) MXene quantum dots [2]. An increase in the no. of edge sites, in the quantum dots serves as potential catalytic sites for hydrogen evolution reaction. Moreover, the reduction of size increases the surface area to volume ratio for the quantum dot, which positively contributes to the superior hydrogen evolution performance.

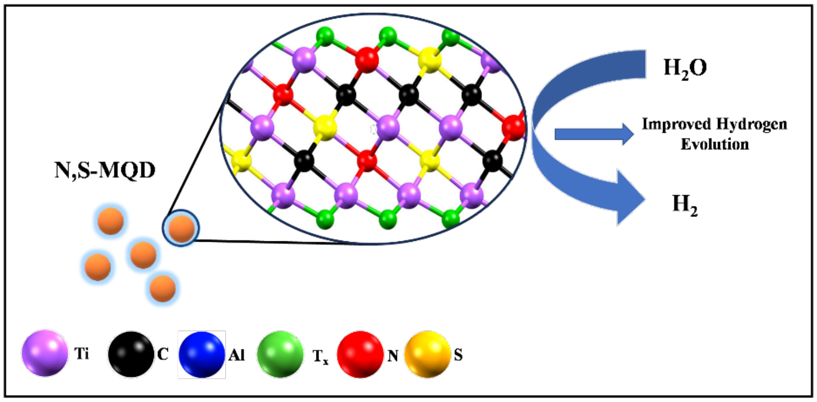

Figure 1. Graphical abstract of the improved hydrogen evolution in N, S-MQD

In this present study, we have developed a heteroatom doped MXene quantum dot (N, S-MQD) via hydrothermal route. The physiochemical structure of the MXene quantum dot has been investigated by FTIR, TEM, XPS and Zeta potential analysis. The N, S-MQD serves as an efficient electrocatalyst for HER. It shows a minimum overpotential of 116 mV to attain the cutoff current density of 10 mA/cm^2, surpassing the performance of currently available electrocatalyst systems based on quantum dots. The incorporation of heteroatom as nitrogen and sulfur in the MXene matrix modulates the electronic structure of the material. This synergistic effect of both the factors mentioned above multiplies the performance significantly. We believe that this work will open a new horizon of quantum dot based electrocatalyst systems.

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P-30

Selective and Sensitive Sensing of Nicotine and its Metabolite Cotinine by Fe(III) Metal-Organic Framework Nanospheres and Its Application in Live-Cell Imaging

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Nicotine, a significant component of cigarette smoke and secondhand smoke (SHS), poses serious health risks due to its carcinogenic potential.[1] Cotinine, the primary metabolite of nicotine, provides a direct measure of human exposure to SHS.[2] Therefore, there is a pressing need to develop a sensing platform that can simultaneously detect nicotine and cotinine to promote environmental safety and protect human health. Metal-organic frameworks, as a novel class of porous crystalline materials, show immense potential for functional modification and optical sensing.[3] Therefore, a novel iron (III) metal-organic framework (Fe-MOF) nanosphere with the formula $[Fe_3(\mu_3\text{–}O)(C_7O_2H_5)_6(COO)_2(H_2O)\cdot 2DMF]$ was synthesized via a solvothermal method.

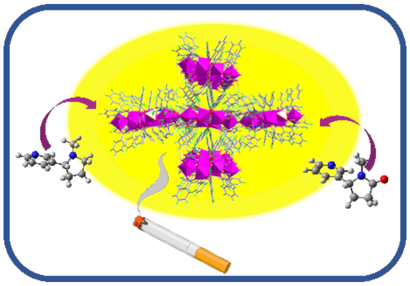

Figure 1. Graphical abstract of the nicotine and cotinine sensing by Fe-MOF.

This Fe-MOF exhibits significant potential for the selective turn-on sensing of nicotine and its principal metabolite, cotinine. The Fe-MOF compound is highly selective for the fluorogenic detection of nicotine and cotinine, even in the presence of interfering and other biologically relevant analytes. The fluorescent probe displayed extraordinary sensitivity for nicotine and cotinine (detection limit 1.1 µM and 1.7 µM) in an aqueous medium. Density functional theory (DFT) calculations and ultraviolet-visible (UV–vis) absorption studies have shed light on the likely sensing mechanism. Taking advantage of its high selectivity and sensitivity for nicotine and cotinine, the probe was successfully employed to image intracellular analytes. Imaging studies with A549 cells revealed the emergence of bright green fluorescence after loading with subsequent treatment with nicotine and cotinine solution.

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P-31

Enhanced Detection of 4-Nitrophenol Using a Synergistic SERS Effect of AgNPs/NiOMFs Composite on a Flexible Substrate

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This study presents the development of a novel SERS substrate that combines silver nanoparticles with nickel oxide microflowers (AgNPs/NiOMFs) on a filter paper (FP) platform, tailored for detecting the priority pollutant, 4-nitrophenol (4-NP). The fabrication process of the AgNPs/NiOMFs@FP substrate involves a simple two-step procedure: the hydrothermal synthesis of NiOMFs directly onto the FP, followed by photoreduction to deposit AgNPs. The NiOMFs create a three-dimensional hierarchical architecture that hosts a high density of AgNP hotspots, which significantly boosts the Raman signal. Additionally, the interaction between Ag and NiO supports effective electron transfer, further enhancing the SERS performance. This advanced AgNPs/NiOMFs@FP substrate demonstrates notable attributes, including excellent reproducibility (with a relative standard deviation of 7.54%), uniform signal distribution, and long-term stability, retaining 70% of its efficiency after 12 days.

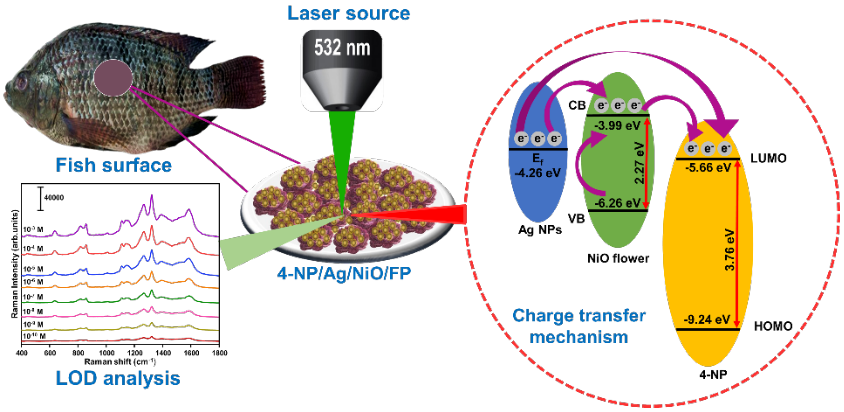

Figure 1. Graphical abstract for the SERS detection of 4-NP from fish surface.

The flexible SERS substrate can detect 4-NP, achieving a low detection limit of 3.32 × 10^{-12} M and an enhancement factor of 3.39 × 10^{9}. Its flexibility allows for precisely detecting 4-NP across diverse samples, such as tap water, river water, and fish surfaces. The straightforward preparation process, coupled with exceptional analytical capabilities and practical applicability, makes the AgNPs/NiOMFs@FP substrate a valuable tool for environmental monitoring and food safety. The study emphasizes the crucial role of the AgNPs/NiOMFs composite in enhancing SERS sensitivity. The unique three-dimensional structure of the NiOMFs provides abundant AgNP hotspots, while the synergistic interaction between Ag and NiO promotes effective electron transfer, collectively creating a highly sensitive detection platform. The AgNPs/NiOMFs@FP substrate offers a promising approach for monitoring environmental pollutants and ensuring food safety.

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P-32

NNN-Pincer Chromium Catalysed Dehydrogenative Synthesis of 3-Oxo and 3-Amino Quinoline Derivatives Using *β*-O-4′ Lignin Models or α-Amino Ketones.

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Quinoline represents a widely occurring structural motif in numerous important drug molecules. Many methods have been developed for the synthesis of quinoline derivatives. The Friedländer methods represents a general synthetic procedure for 2-substituted quinoline, proceeding by cyclization reaction between 2-amino benzaldehyde and ketones. Due to unstable property of 2-aminobenzaldehyde, catalytic dehydrogenation involving tandem reaction using 2-aminobenzyl alcohol instead exhibit more advantages. Transition metal catalysed synthesis of quinoline derivative from 2-aminobenzyl alcohol is an efficient and sustainable approach.

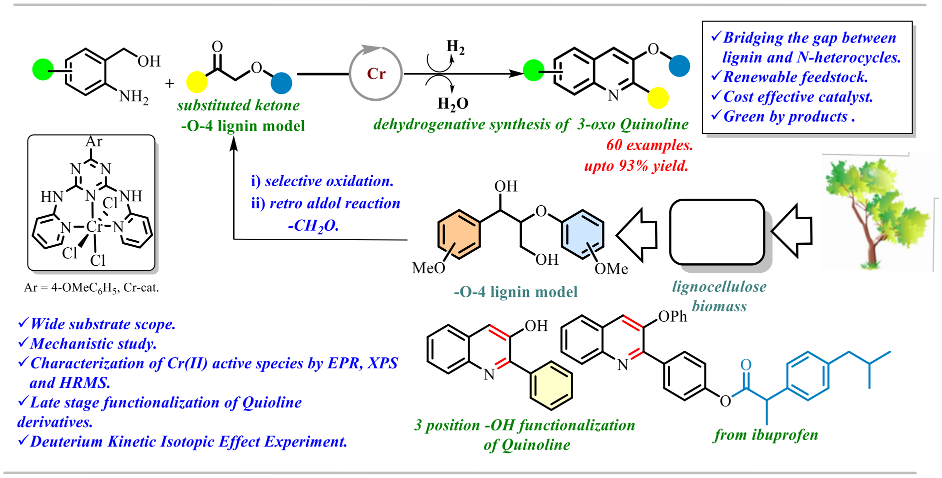

Figure 1. Graphical abstract of Synthesis of 3-Oxo and 3-Amino Quinoline Derivatives.

Here in we report an efficient Chromium catalysed acceptorless dehydrogenative annulation of 2-aminobenzyl alcohols with active methylene bearing ketones, phenoxy acetophenone as *β*-O-4′ lignin model. Lignin, a highly abundant aromatic polymer in plant cell walls, and the β-O-4′ linkage is the most abundant which constitutes 50-80% of the interunit linkages. The reaction provides an efficient route for the construction of 3-oxo substituted quinolines *via* acceptorless dehydrogenative coupling (ADC) reaction using an earth abundant metal without the need of any external chemical oxidant or additives. Interestingly, this catalytic route gives a unique opportunity to provide hydroxyl motif at the C3-position of the heteroaromatic moiety which otherwise can be achieved by hydroxyl group incorporated at the C3 position *via* *N*-oxide using aryldiazonium salt. Notably, the synthetic applicability of the present protocol is further extended towards the synthesis of 3-aminoquinoline derivatives. Mechanistic study of the reaction has been done by different competitive reactions, Deuterium kinetic isotope effect (DKIE) experiment and the in-situ generated Cr (II) active species has been characterized by EPR, XPS and HRMS.

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P-33

Screening of Pyrimidine Derivatives for DGAT1 inhibition, a Cure for Obesity through Computational tools.

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In recent years, obesity has become a global problem, leading to other diseases such as fatty liver disease, type 2 diabetes, and heart disease[1]. The accumulation of triglycerides in the human body is one of the primary causes of obesity. DGAT1 (diacylglycerol acyltransferase 1) is a membrane protein that plays a crucial role in the synthesis of triglycerides and is a potential therapeutic target for obesity[2]. Pyrimidine is a heterocyclic compound known for its broad-spectrum biological activities, while morpholine plays a diverse pharmacological role[3][4]. It's worth noting that numerous DGAT1 inhibitors incorporate pyrimidine and morpholine moieties in their structures[5][6] and we emphasize morpholine-containing pyrimidine compounds because of their ability to enhance pharmacokinetic properties[5]. Taking inspiration from its medicinal history, we screened morpholine-fused/linked pyrimidine compounds using several computational methods to study their effectiveness against the target DGAT1 target protein (PDB ID: 6VP0). A library of 250 Pyrimidine derivatives from the Zinc database and Pubchem was created. Autodock Vina was used to conduct molecular docking of the ligands against the target protein and obtained a binding energy range of - 6.0 to -11.6 kcal/mol. The ADME properties and bioactivities were analyzed using Molinspiration and PreADMET server, which provided the top 20 leading compounds. A 2D-QSAR model was built using known DGAT1 inhibitors, and the pIC50 values for our top 20 ligands were predicted that closely match known inhibitors. The top two leading compounds were also subjected to molecular dynamics simulations on Gromacs for 100 nanoseconds to assess the stability of the ligand-protein complex. Principal component analysis (PCA) and MMPBSA study were also conducted. Moreover, the results were compared with the well-known DGAT1 inhibitor T-863, and promising results were found, suggesting potential for future treatments. A detailed analysis of our results will be discussed at the symposium.

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P-34

Electrochemical analysis of C-Reactive Protein for Diagnosis of CVDs by using Ni-doped Copper Ferrite Nanoparticles

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In preasents work Ni-doped copper Ferrite (Ni$_x$CuFe$_{x-2}$) nanoparticles were synthesized by hydrothermal process at different concentrations of Ni (0.05, 0.10,.0.15, 0.20) using ***Magnolia grandiflora*** leaf extract. their structure and properties were studied through FT-IR, X-ray, XRD, SEM, UV, and XPS. XRD confirmed the crystalline size of nanoparticle which was in the range of 17-34 nm. FTIR at 437 cm^{-1} to 635 cm^{-1} confirms spinel ferrite structure , vibration band at 490 cm^{-1} is due to tetrahedral and octahedral ferrite. 1120 cm^{-1} are associated with the bond formation during synthesis of copper ferrite and 1390 cm^{-1} band stretching vibration of the nitrate. ITO electrode was fabricated with synthesized nanoparticles by Electrophoretic deposition (EPD) method and then Electrochemical sensing was done by Cyclic voltammetric (CV), Electrochemical Impendence study (EIS) the detection CRP biomarkers in the range of **0.5 ng/ml** to **5µg/ml.** during electrochemical analysis, though the graph obtained I/E (current/potential),obtine is linear.

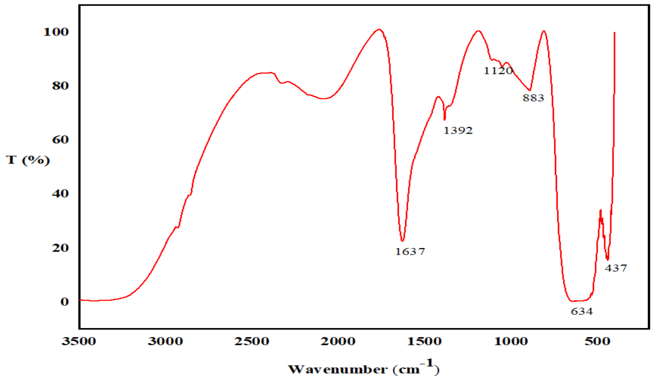

Fig. FTIR graph of the synthesized Ni- doped Copper Ferrite nanoparticles

Keyword- *Magnolia Grandiflora***,** Ni-doped copper Ferrite, EPD, cyclic voltammetric, EIS, CVDs

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P-35

Synthesis of phenylethanoid glycosides from acrylic esters of glucose and aryldiazonium salts *via* palladium-catalyzed cross-coupling reactions and evaluation of their anti-Alzheimer activity

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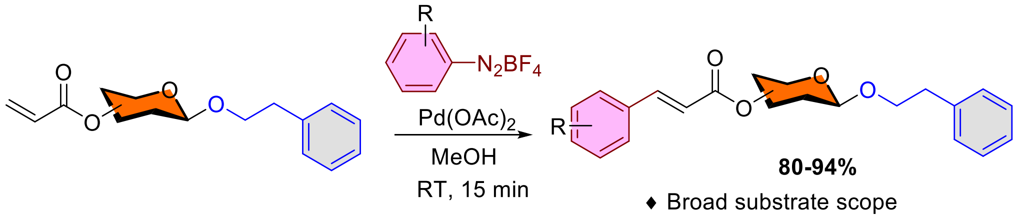
Synthesis of *trans*-cinnamic acid containing glucosides (i.e. derivatives of phenylethanoid glycosides) was achieved *via* palladium-catalyzed cross-coupling reactions between glycosyl acrylic esters and aryldiazonium salts. A wide range of functionalized aryl diazonium salts underwent coupling reactions with 6-*O*-and 4-*O*-acrylic esters of glucose in the presence of palladium acetate, while the desired compounds were obtained in good to excellent yields. The reactions proceed at room temperature in the absence of additives and base. Selected compounds from the library were screened for anti-Alzheimer activity, while one of the compounds from the library displayed significant inhibitory activities against butyrylcholinesterase (BChE) and acetylcholinesterase (AChE) enzymes.



- ♦ Broad substrate scope
- ♦ Short reaction time
- ♦ Milder reaction conditions
- ♦ Excellent yields
- ♦ Room temperature
- ♦ Anti- Alzheimer activity

Figure 1. Synthesis of cinnamic acid ester of phenylethanoid glucosides

Considering the position of cinnamic acid groups in naturally occurring phenylethanoid glycosides the model substrates of 6-*O*-acrylic ester and 4-*O*-acrylic ester were designed and synthesized. Further, we investigated the optimization of cross-coupling reaction using 6-*O*-acrylic ester with different aryl donors in the presence of a palladium catalyst. Having explored the scope of the reaction between 6-*O*-acrylic ester of glucose and aryldiazonium salts, we further investigated the coupling reaction between 4-*O*-acrylic ester of glucose and aryldiazonium salts under optimized conditions. Then, after exploring the synthesis of various 6-*O* and 4-*O* cinnamyl esters of glucose derivatives, we investigated the synthesis of cinnamyl esters containing phenylethanoid glucosides. From the library, selected compounds were screened for anti-Alzheimer activities while one showed significant inhibitory activities against butyrylcholinesterase (BChE) and acetylcholinesterase (AChE) enzymes.

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P-36

Synthesis, structural insights and catalytic activity of diorganotin(IV) complexes with pincer ligand

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Applications of structurally vibrant organotin compounds in numerous fields cover a wide spectrum of biological applications and catalytic activity [1-2]. Organotin (IV) compounds as catalyst have also reached distinct statures due to, in a great extent, absence of side reactions, good efficiency even under mild conditions, and encouraging toxicological and environmental properties [2]. Therefore, they have been employed as industrial catalysts for esterification, polyvinyl chloride (PVC) stabilization, and their use as catalyst continues to appear in the literature [3-4].

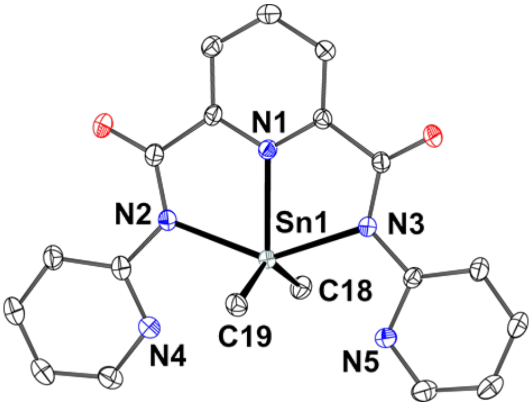

Figure 1. Displacement ellipsoid plot of a molecule in the crystal structure of **1**·0.5C_6H_6

Diorganotin (IV) complexes of composition [R_2SnL] (R= Me (**1**·0.5C_6H_6), *n*-Bu (**2**), Bz (**3**)) were synthesized by reacting appropriate diorganotin oxides with the tridentate pyridine dicarboxamide ligand (H_2L). The structures of the compounds **1-3** were determined in solution by ^{1}H, ^{13}C, ^{119}Sn NMR in $CDCl_3$, and HRMS in acetonitrile solvent. The molecular and crystal structures of **1**·0.5C_6H_6 (Figure 1), **2**, and **3** were determined using single-crystal X-ray diffraction analysis (SCXRD). ^{119}Sn NMR spectroscopy, revealing that the complexes adopt a five-coordinate structure in a non-coordinating solvent. SCXRD results indicated that the rigid tridentate pyridine dicarboxamide ligand and the Sn coordinating C atoms adopt nearly C_2v symmetry and thus match none of the most popular geometries for five-coordinated species, namely square pyramidal or trigonal-bipyramidal coordination. Results pertaining to synthesis, characterization and catalytic activity of ε-caprolactone formation via Baeyer-Villiger oxidation of cyclohexanone will be presented.

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P-37

Chirality-Directed Diversity in the Morphology of Dipeptides and Sensing of Fe^{3+}

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Molecular self-assembly is a method for creating groups of nanostructures, where molecules independently organize themselves through various noncovalent interactions e.g. van der Waals forces, electrostatic interactions, hydrogen bonding, π−π stacking, and hydrophobic interactions.[1] Supramolecular self-assembly using small peptides has garnered significant interest due to its chemical diversity, cost-effectiveness, and ease of modification compared to other molecules.[2] Peptide self-assembly can produce a variety of nanostructures depending on internal and external forces.[3] These peptide nanostructures generally possess excellent biocompatibility, low toxicity, low immunogenicity, biodegradability, and target specificity. As a result, they are widely used in drug delivery, tissue engineering, biomedical applications, cell culture, nanoelectronics, and sensors. Moreover, nanostructures like nanotubes and fibrillar structures play crucial roles in practical applications.[4] The chirality-controlled self-assembly of two small dipeptides was examined. The N-terminal Fmoc and C-terminal methyl ester-protected dipeptides Fmoc-L-Ala-L-Val-OMe (1) and Fmoc-L-Ala-D-Val-OMe (2) formed an intermolecular H-bonded parallel β-sheet structure in the crystalline state.[5] Altering the chirality of Val resulted in different morphologies. In a 1:1 acetonitrile-water mixture, peptide 1 displayed hollow tube structures, while peptide 2 exhibited fibrillar morphology at the micro- to nano-level. These self-assembled structures demonstrated significant thermal stability under dry heating conditions and could bind with bioactive dyes such as thioflavin T, rhodamine B, fluorescein, and 5(6)-carboxyfluorescein. Notably, both peptides selectively detected Fe3+ ions and could serve as fluorescent probes for Fe3+ ions.

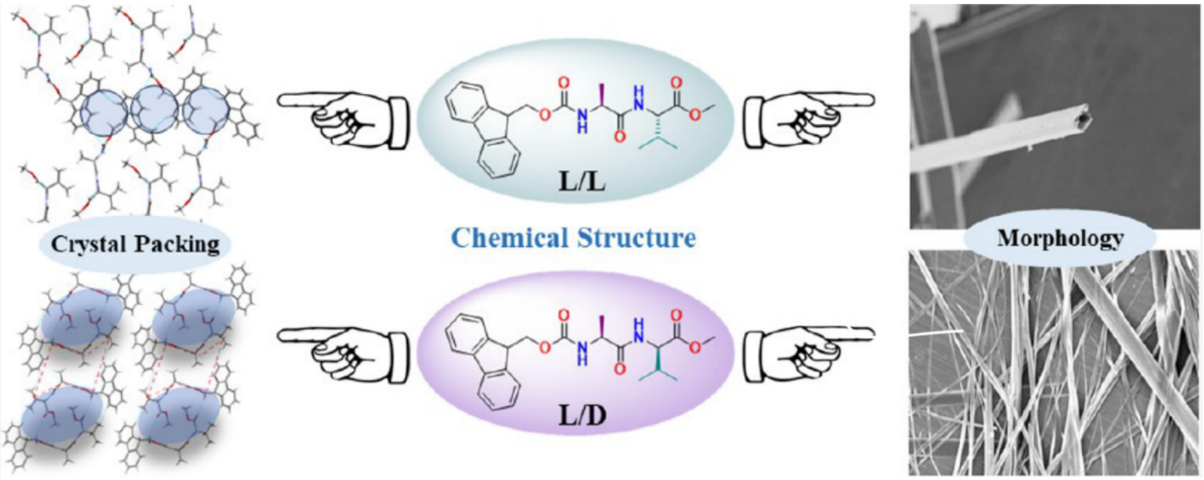

Figure 1 Variation in crystal packing and morphology under the influence of chirality.

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P-38

Production of Lactic Acid via Catalytic Transfer Dehydrogenation of Glycerol Catalyzed by Base Metal Salt Ferrous Chloride and Its NNN Pincer-Iron Complexes

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The synthesis and characterization of a series of four NNN pincer-Fe(II) complexes of the type $(^{R2}NNN)FeCl_2$ (R = Cy, R = ^{t}Bu, R = ^{i}Pr and R = Ph) based on *bis*(imino)pyridine ligands have been discussed here [1]. All the complexes are synthesized under argon atmosphere and observed NNN pincer-Fe(II) complexes with an expected trigonal bipyramidal (TBP) geometry were found to equilibrate to a rearranged ion pair of an octahedral dicationic Fe complex containing two *bis*(imino)pyridine ligands that is neutralized by a tetrahedral dianionic $[FeCl_4]^{2-}$. And we have characterised by SCXRD, HRMS and UV-Vis studies suggests that the equilibrium was mostly dictated by the sterics of the R group on the imine N, with the less crowded groups tilting the equilibrium to the ion pair and the bulky ones favouring the TBP geometry. Combined inference from EPR studies and Evan's magnetic moment measurements indicated that in all the considered pincer complexes, the central Fe(II) in paramagnetic, high-spin state. The same solution was kept open to air for seven days, these pincer-iron complexes are oxidized to a mixture of low-spin and high-spin Fe(III) species. These NNN pincer-Fe(II) complexes were found to be highly active towards the transformation of bio-diesel waste glycerol (GLY) to value-added lactic acid (LA). In this work, acceptorless dehydrogenation of glycerol as well as transfer dehydrogenation of glycerol has been accomplished utilizing a commercially available base metal salt ferrous chloride and its NNN pincer-iron complexes Particularly, $(^{Ph2}NNN)FeCl_2$ (0.1 mol%) gave 91% LA with a 99% selectivity at 140 °C using 1.2 equiv. of NaOH. With 0.0001 mol % $(^{Ph2}NNN)FeCl_2$, very high turnovers (74% LA, 98% selectivity, 740 000 turnover number (TON) at 4405 turnovers per hour (TOs/h)) were obtained after 7 days. EPR indicated Fe(III) species to be the active catalyst, a few of which were detected by HRMS. Few independent experiments with PPh_3 and Hg are suggestive of the major contribution is from homogeneous molecular nature of the catalyst and a minor contribution from heterogeneous Fe-nanoparticles. For these Fe-nanoparticles are further investigated by SEM, TEM, EDX and DLS analysis. A KIE of 1.56 was observed in labelling studies which indicated the involvement of C-H bond activation as a part of the catalytic cycle but not as a part of the rate-determining step.

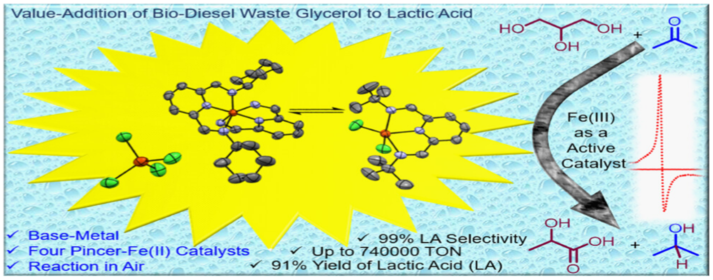

Figure 1. Graphical abstract of the production of lactic acid via catalytic transfer dehydrogenation of glycerol catalyzed by base metal salt ferrous chloride and its NNN pincer-iron complexes.

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P-39

Synthesis of Chitosan-Pectin Based Adsorbent for Efficient Dye Removal from Wastewater

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A green and sustainable approach was used to synthesize chitosan-pectin gel beads (CPBs), which were subsequently applied for the removal of methylene blue dye from aqueous solutions. Cross-linked chitosan-pectin-epichlorohydrin bio-beads were developed as potential biosorbents, aimed at evaluating their effectiveness in treating wastewater, particularly in adsorbing and eliminating methylene blue dye pollutants. The structural properties of CPBs were thoroughly examined using SEM, FTIR, and XRD, while their mechanical strength was assessed with a Texture Analyzer. The stability of CPBs was also tested in acidic conditions. Several parameters, including pH, contact time, temperature, initial heavy metal concentration, adsorption mechanism, and regeneration, were systematically studied to gain a comprehensive understanding of the adsorption behavior. Adsorption-desorption experiments validated the excellent reusability of CPBs, highlighting their potential as environmentally friendly and durable adsorbents for the efficient removal of methylene blue dye from water. The adsorption process was found to be both endothermic and spontaneous[1]. The results indicated that the pseudo-second-order model best described the adsorption kinetics, while the Langmuir isotherm model effectively captured the adsorption behavior of grafted cross-linked chitosan-pectin beads. The primary mechanisms involved in the adsorption process were hydrogen bonding, electrostatic attractions, and n-π stacking interactions[2].

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P-40

Metal-Free Multi-fold Thioetherification of Aryl Halides

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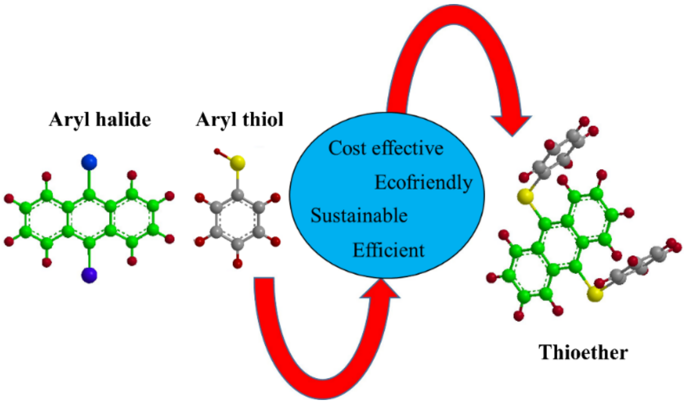
Thioethers are widely distributed in nature and are found in numerous bioactive compounds.[1] In addition, thioethers are significant class of motifs with extensive implementation in biological chemistry, drug design, organic synthesis and material science.[1] As a result over the past few decades, the synthesis of thioethers has sparked a lot of fascination. Transition metal catalysed thioetherification of aryl halides with thiols is a potent technique for the synthesis of thioethers that are typically accomplished in the presence of light or under thermal conditions. The cross-coupling reaction between aryl halides and thiols employing $Pd(PPh_3)_4$ as a catalyst was first reported by Migita and co-workers in 1980.[2] Beyond Pd-based metal catalysts, other transition metal based catalytic systems based on nickel, iron, cobalt, rhodium, manganese and gold have also been explored for the construction of C-S bonds.[1] However to achieve good reactivity, transition metal catalytic methods often require a high catalyst loading, a strong base and a robust ligand system.[3] Herein, we have reported a new approach towards the multi-fold thioetherification that is accomplished under transition metal-free conditions using readily available green solvent. This protocol offers easy handling, mild reaction conditions and a sustainable way to synthesize aromatic thioethers from aryl thiols when coupled with unactivated aryl halides. The newly formulated metal-free thioetherification reactions have been studied in detail from a synthetic and mechanistic point of view.



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P-41

Redox switchable palladium catalyzed cross coupling of aryl boronic acids with aliphatic anhydrides

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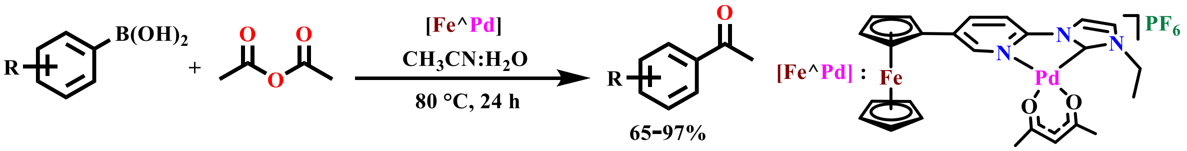
Redox switchable catalysis has gained significant interest since it offers unique approach to controlling chemical reactivity in various organic transformations. Switchable catalyst employs the ability of a catalyst to change its oxidation state, which in turn modulates its electronic properties and, consequently, its catalytic behavior.[1] It gives a distinct state to a catalyst where it can display a different kind of activity, selectivity or some other specific properties.[2] In the design of bimetallic complexes, the increasing recognition of the ferrocene moiety as a redox-switchable metallo-ligand, due to its reversible and easy Fc/Fc$^+$ redox change, along with its synthetic flexibility and high stability, highlights its potential applications in catalysis and makes it an ideal candidate for incorporation into ligand systems.[3] In recent years, there has been significant progress in cross-coupling reactions facilitated by palladium complexes featuring ferrocenyl substituents. In this context, we envisaged incorporating a ferrocene unit in our N-heterocyclic carbene (NHC) based ligand system and synthesized a palladium complex and its oxidized version to explore the catalytic activity of both the complexes in the acylative coupling of arylboronic acid and acetic anhydride to obtain aryl ketone in phosphine, base and additive free conditions with the production of a minimum amount of waste.

Following the successful synthesis of aryl ketones, we further explored the synthetic potential of trifluoromethyl ketones, a crucial class of organofluorine compounds with immense potential in drug design and development. This was achieved using our ferrocene-decorated NHC palladium complex with redox switchable properties which facilitates the trifluoroacylative coupling of arylboronic acid and trifluoroacetic anhydride via C–O bond cleavage under solvent-free conditions.

Figure 1. Acylative cross coupling of arylboronic acid and acetic anhydride



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P-42

Exploring Solvent-Driven Disorder and Magnetism: Systematic Study of Alkaline Earth Metal-Formate Frameworks

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This study presents a comprehensive analysis of alkaline earth metal formate frameworks (MFFs), focusing on their solvent-dependent structural transformations at room temperature. The MFFs were synthesized by formates acting as linkers generated by in-situ[1] decomposition from DMF under various conditions, forming crystals with the molecular formula A_2BX_3,[2] where A represents a disordered species, B denotes metal ions, and X corresponds to formates. Our investigation revealed a notable solvent-assisted crystal-to-crystal change from the triclinic (space group: *P1*) of parent crystal (MFF 101) to a rhombohedral (*R*3*c*) (MFF 102) in ethanol to tetragonal structure ($P4_32_12$) (MFF 103) in chloroform and imidazole and to Monoclinic ($P2_1/c$) (MFF 104) with Toluene. These transitions, observed at room temperature, highlight the tunability of the framework, a unique feature for alkali earth metals.

The study also explores the role of formic acid as a linker and C_2N_3[3] as a disorder within the MFF topology, elucidating how solvent interactions influence the disorder and stability of the framework. One of the key findings is the near room temperature (291 K) magnetic behaviour exhibited by these MFFs, which is rare for alkaline earth metal frameworks. This magnetic behaviour, combined with the high selectivity for CO_2 adsorption over N_2, positions these materials as promising candidates for various applications.

The ability to control the disorder within the framework through solvent interactions opens up opportunities for designing MFFs with tailored properties, offering a deeper understanding of the underlying chemistry and structural dynamics of trapped disorders and paving the way for innovations in material design.

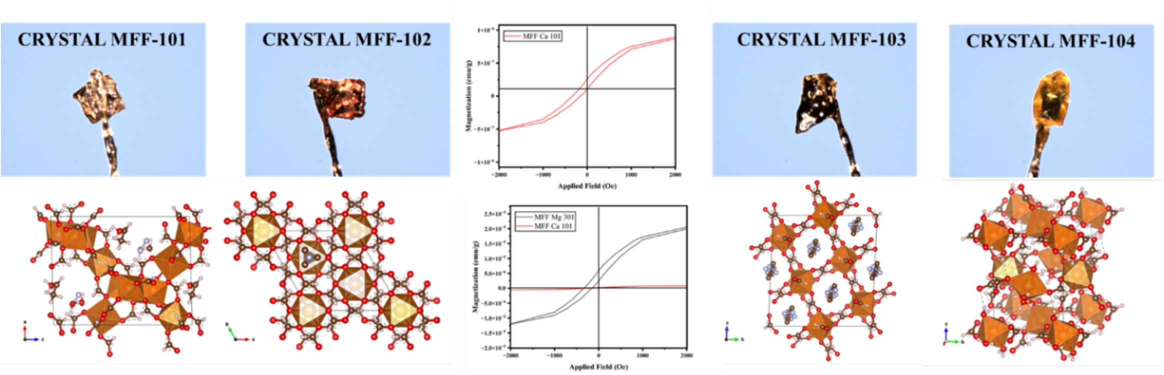

Figure 1. Solvent assisted crystal to crystal transformation in alkaline earth metals-formate framework and magnetic behavior.

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P-43

Enantioselective synthesis of *α, α'*-disubstituted *α*-amino acid derivatives *via* conjugate addition of *α*-nitroesters to vinyl sulfones

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A sulfur atom containing quaternary α-amino acid derivatives play a crucial role in designing life as well as acting as a building block for the synthesis of various peptides and proteins. Moreover, the presence of quaternary α-amino acid moieties on peptides increases their resistance ability against chemical and enzymatic degradations.[1, 2] In addition, the introduction of sulfone moiety in amino acid scaffold significantly influences biological activity as chiral sulfone derivatives have a higher propensity of hydrogen bonding which would have a substantial impact on the efficacy and potency of the intended biological target. On the other hand, chiral sulfone-containing drugs are effective for the treatment of diseases such as dermatitis herpetiformis, tuberculosis, and leprosy. They also have other therapeutic properties including antimicrobial, anti-inflammatory, anti-HIV, anticancer, antimalarial, etc. Therefore, the development of complementary strategies for synthesizing these quaternary enantioenriched valuable chiral compounds has drawn attention in the past few decades.[3, 4] Herein, we report the synthesis of diversified enantioenriched quaternary Michael adducts of α-nitroesters bearing sulfone moiety under metal-free conditions utilizing easily accessible vinyl sulfones and well-known amino acid precursor α-nitrocarboxylates, in the presence of a cinchona-based chiral catalyst. This methodology offers a convenient avenue for synthesizing Michael adducts that are employed as a α-amino acid precursor with outstanding yield, moderate to excellent enantioselectivity, good functional group tolerance, and synthetic utility.

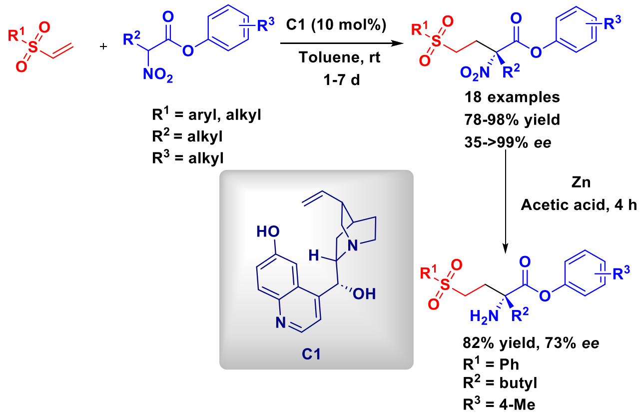

Figure 1. Graphical abstract of the synthesis of enantioenriched amino acid derivatives

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P-44

Palladium-Catalyzed Annulative Coupling of Spirovinylcyclopropyl Oxindoles with *p*-Quinone Methides

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In this article we have reported Pd-catalyzed annulative coupling of spirovinylcyclopropyl oxindoles with *p*-quinone methides has been accomplished *via* cascade carbon-carbon bond formation to afford bis-spirooxindole scaffolds (Figure 1). The mild reaction conditions, diastereoselectivity, functional group diversity, post-synthetic transformations and mechanistic studies using DFT calculations are the important practical features. The details will be presented during the conference.

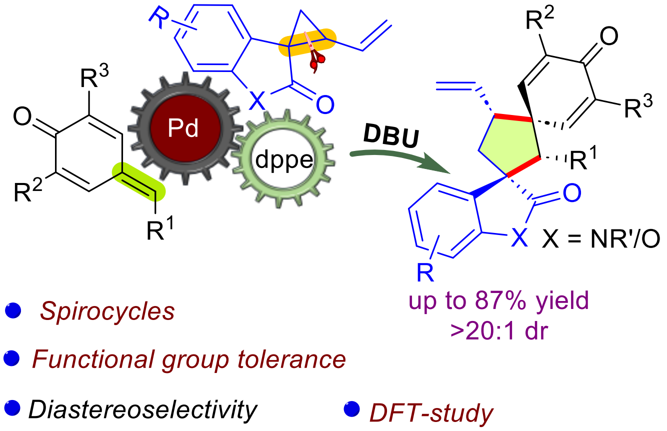

Figure 1. Synthesis of bis-spirooxindoles

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P-45

Amine-functionalized magnetically recyclable demulsifier for efficient separation of crude oil-water emulsion

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The fluids produced from an oil well typically emerge as a complex blend of crude oil, water, and natural gas. These fluids undergo separation into distinct phases at surface processing facilities through several stages. Following the initial separation of gas and free water, crude oil remains in the form of an emulsion, often containing up to 15% water.[1,2] To meet regulatory requirements prior to being delivered to end consumers, these water-in-oil emulsions must undergo demulsification. The most common demulsification method involves the use of chemical demulsifier in conjunction with heat treatment.[3-6]

This study explores the fabrication of a class of functionalized core-shell magnetic nanomaterial *viz*, amine-functionalized V_2O_5 nanoparticle coated Cobalt ferrite ($CoFe_2O_4$) and polydiallyldimethylammonium chloride (PDDA) grafted amine-functionalized V_2O_5 nanoparticle coated Cobalt ferrite denoted as $CoFe_2O_4@V_2O_5\text{-}NH_2$ and $CoFe_2O_4@V_2O_5\text{-}NH_2@PDDA$ respectively for crude-water demulsification process. The two nanomaterials were synthesized by co-precipitation method followed by surface modification with (3-aminopropyl) triethoxysilane (APTES) in the presence of varying concentrations of V_2O_5 nanomaterial and PDDA. The $CoFe_2O_4@V_2O_5\text{-}NH_2$ and $CoFe_2O_4@V_2O_5\text{-}NH_2@PDDA$ nanoparticles were characterized by X-ray diffraction, transmission and scanning electron microscopies, fourier transform infrared spectroscopy, thermogravimetric−differential thermogravimetric analyses, and vibrating sample magnetometry. Demulsification efficiency was assessed through traditional bottle tests. The demulsification tests were carried out for a wide range of emulsions containing varying amounts of water content at various temperature settings and varied pH levels to validate the efficiency of the prepared nanomaterials. Also, the nanomaterials were incorporated at different concentrations to determine the optimal dosage. Results indicate that both nanocomposites effectively demulsified stable water-in-crude oil emulsions across all temperatures, achieving complete separation within 10 minutes. Additionally, $CoFe_2O_4@V_2O_5\text{-}NH_2$ nanoparticles displayed notable magnetic recyclability, maintaining high demulsification efficiency even after multiple recycling cycles with minimal degradation. Functionalized magnetic nanomaterial coated with Vanadium pentoxide for demulsification of crude oil is used for the first time.

Keywords: Crude oil; demulsification; emulsion; nanoparticle

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P-46

Enhanced Energy Harvesting Using a TiO_2/NiO Heterojunction via Direct Semiconductor Interface

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The intentional insertion or manipulation of defects in materials at atomic level or nanoscale, referred to as defect engineering has a key role in the modification or improvement of physical, chemical and electrical characteristics of materials. This study investigates a unique method for energy harvesting by fabricating a direct semiconductor heterojunction with doped n-type and p-type materials. Titanium dioxide (TiO_2) was chosen as the n-type semiconductor, doped with nitrogen to augment its n-type characteristics, while nickel oxide (NiO) served as the p-type semiconductor, doped with iron to reinforce its p-type capabilities. The p-type and n-type materials are subsequently combined to form a heterojunction and copper tape electrodes were affixed to both sides to establish electrical contacts. A high open circuit voltage of about 35 V and current of about 100 nA at 30% RH and 25 °C from one such single device underscored the potential of this heterojunction for energy harvesting applications. This methodology presents a novel perspective in the sector, as it utilizes a direct semiconductor heterojunction for the generation of power, unlike typical photovoltaic approaches. The successful increase of the n-type and p-type behaviours via doping, together with the development of the heterojunction, provides possibilities for new energy harvesting devices, enabling a cost-effective and scalable way for applications like lighting up an LED and powering up a calculator.

P-47

Stimuli-responsive assembly and disassembly of anionic suprasomes with tunable antibacterial activity

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Host–guest complexation-based suprasomes successfully deliver benzimidazolium amphiphiles. β-CD and Zn^{2+} or an acidic environment act as the stimuli for the assembly and disassembly of suprasomes. We developed host–guest complexation-based suprasomes to deliver cationic amphiphiles and antibiotics. The β-CD-mediated formation of suprasomes with negative surface potential from the mixed micelles of cationic and anionic amphiphile could also release the encapsulated cargos in a stimuli-responsive manner in the presence of Zn^{2+} or an acidic environment. The superior activity of tetracycline-encapsulated suprasomes in the presence of Zn^{2+} ions could be due to the combined effect of cationic amphiphile, tetracycline, and Zn^{2+} ions against Gram-positive *S. aureus* bacterial cells. The hemolytic assays showed that the selected formulation has lower toxicity against RBCs. Therefore, the multi-stimuli regulated step-wise transition of micelles suprasomes-other aggregates is of great interest in drug delivery. In addition, facile functionalization and stimuli-responsiveness could provide suprasomes as the next-generation drug delivery systems to combat bacterial infections, cancer, and other diseases.[1]

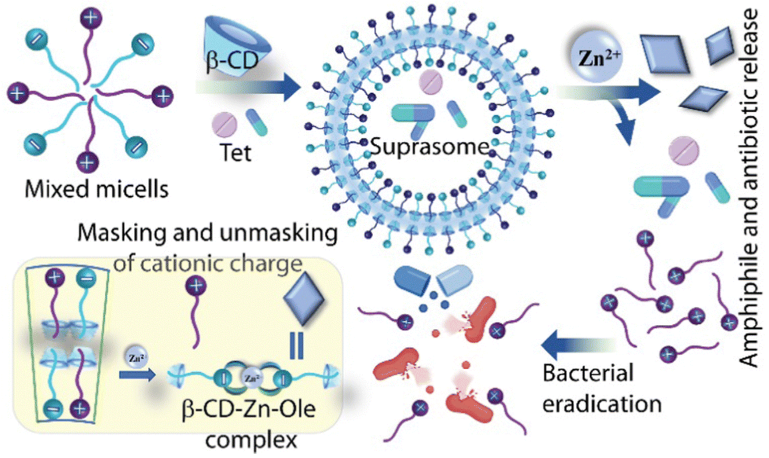

Figure 1. Graphical abstract of stimuli-responsive assembly and disassembly of suprasomes with antibacterial activity.

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P-48

Bithiophene Conjugated Naphthalenylmethanone: Facial Synthesis and Photophysical Properties

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Molecules with a twisted donor-acceptor (D-A) architecture are widely employed to develop materials with aggregation-induced emission (AIE), which are essential for developing innovative biological sensors, solid- state emitters, and stimuli-responsive materials [1]. In good solvents, luminogenic materials remain non- emissive and exist in their molecular form. However, in poor solvents, these molecules aggregate and become highly luminous. Luminates exhibiting AIE are termed AIEgens [2-3]. Aggregation-induced emission (AIE) luminogens (AIEgens) have diverse and valuable applications across various fields due to their unique emission properties, especially in solid states and aggregate forms (Figure 1).

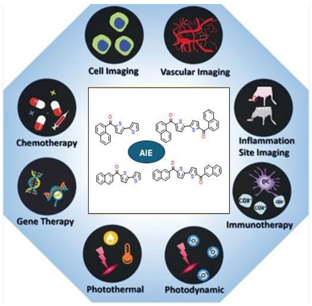

Figure 1. Applications of Aggregation-Induced Emission Luminogens (AIEgens)

We report the design, synthesis, and AIE properties of a novel series of bithiophene-conjugated naphthalenylmethanones. These compounds were synthesized through a simple one-pot reaction between 2,2′-bithiophene and 1-naphthoyl chloride or 2-naphthoyl chloride, catalyzed by $AlCl3$. The resulting compounds (1-3) were fully characterized using multinuclear NMR spectroscopy and mass spectrometry. These flexible compounds exhibit weak fluorescence in solution but demonstrate strong emission in condensed and solid states, with significant AIE enhancement in water/THF mixtures.

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P-49

Cu(II) complex of bidentate pyrazole ligand: A synthetic model for copper nitrite reductases (CuNiR)

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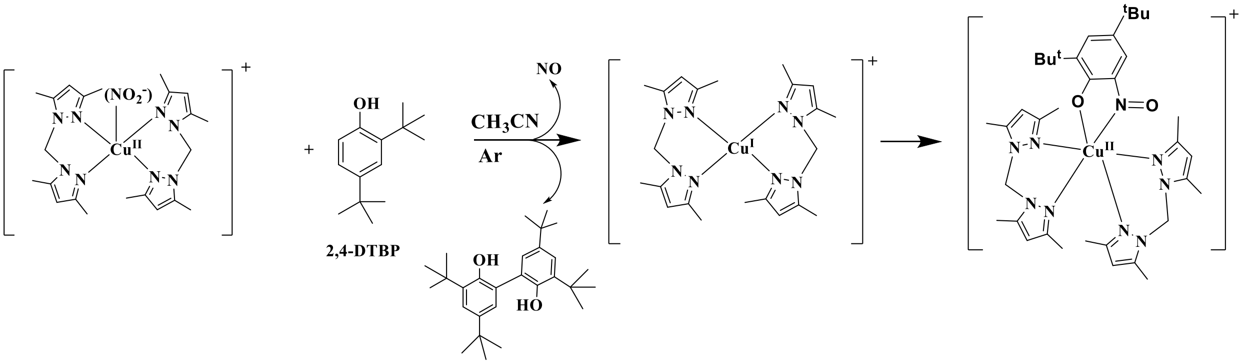
Transition metal ion mediated conversions of nitrate (NO_3^-) and nitrite (NO_2^-) ions to nitric oxide (NO) and nitrous oxide (N_2O) are of immense importance from biochemical and physiological point of view.[1] Understanding of these transformations are important to develop the strategies for enhancing the 'N' content in soil while suppressing the NO_x induced pollution.[2] One of the major steps in these transformations is reduction of nitrite to nitric oxide by nitrite reductase enzymes (NiR).[3]

A model complex, $[Cu^{II}(L)(NO_2)](ClO_4)$, **1** {L= bis(3,5-dimethyl-1H-pyrazol-1-yl)methane} of CuNiR enzyme was synthesized using pyrazole based bidentate ligand framework (L) which effectively converts NO_2^- to NO. The NiR activity of the complex was studied in the presence of 2,4-di-tertiarybutylphenol (2,4-DTBP) as H^+ and e^- source. The formation of NO was confirmed by it's reaction with $[Fe^{II}(dtc)_2]$ {dtc = diethyldithiocarbamate). The involvement of the metal center in the reaction was evident from isolation and structural characterization of the intermediate Cu(I) complex, $[Cu^I(L)](ClO_4)$.



Scheme 1. CuNiR activity of $[Cu^{II}(L)(NO_2)](ClO_4)$ in presence of 2,4-DTBP.

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P-50

Metal interconnected transition metal dichalcogenides meets conducting polymer arrays to give an efficient and stable cathode material for asymmetric hybrid supercapacitors

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Energy is one of the most important needs of the human race; Nowadays, the demand in energy storage devices, as well as the need for a green environment, has become a major global force in past years. In recent decades, hybrid supercapacitors (SC) pay an attention of quick charge and discharge device, which shows advantages such as fast rechargeable feature and extreme energy output.[1] Generally, Various materials such as metal oxides, metal organic frameworks (MOFs), covalent organic frameworks (COFs), conducting polymers (CPs), metal chalcogenides, etc exhibits pseudocapacitance. Contemporarily, researchers have increasingly focused on transition metal dichalcogenides (TMDs) and CPs due to their excellent performance in supercapacitors and other energy storge applications.[2] Additionally, this approach offers the potential for scalable and eco-friendly material synthesis, supporting the development of sustainable energy technologies The versatility of transition metal-TMDs hybrids highlights their crucial role in the advancement of supercapacitors.

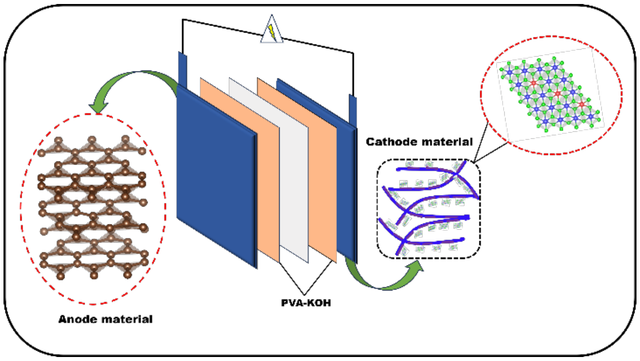

Figure 1. Graphical abstract of the fabricated device.

We present an innovative hybrid electrode material, Metal doped TMDs/conducting polymer(N-VP), synthesized through a sustainable hydrothermal strategy. By systematically adjusting the M1 and M2 precursor concentrations (5:95, 10:90, 15:85) with the constant polymer, we produced three distinct N-VP variants, namely 5N-VP, 10N-VP and 15N-VP each having unique morphological features. Among these, the optimized 15N-VP variant exhibited excellent crystallinity and a branched rodlike structure, delivering a high specific capacitance of 1047.9 F/g at 1 A/g. Furthermore, it maintained 90.52% of its initial capacitance even after 5,000 charge-discharge cycles, underlining its long-term electrochemical stability. To evaluate the capabilities of 15N-VP, we fabricated a hybrid material asymmetric supercapacitor (HMASC) device. The device unveiled admirable energy-storage performance, with a specific capacitance of 30.5 F/g at 1 A/g, power density of 870.87 W kg^{-1} and an energy density of 34.31 W h kg^{-1}. Additionally, it maintained 92.17% of its capacitance even after 10,000 cycles, highlighting its durability and longevity. These results indicate the N-VP hybrid material as a highly promising candidate for future supercapacitor technologies, offering an ideal balance between high energy and power density along with superior cycle stability.

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P-51

Evaluation of Insecticidal Activity of Cycas Leaf Extracts against the Brown Planthopper (*Nilaparvata lugens*) on Rice Cultivation

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Rice (*Oryza sativa*) is one of the staple crops, widely cultivated in the regions of West Bengal, Punjab, Telangana, Odisha, Tamil Nadu, Chhattisgarh, Andhra Pradesh, Bihar, and Assam [1]. However, rice production is significantly threatened by *Nilaparvata lugens* (the brown planthopper), which is responsible for damaging over 10% of rice crops [2]. To address this challenge, the present study investigates the utilization of plant-based natural pesticides, which offer environmental safety and reduced toxicity compared to conventional chemical insecticides such as Imidacloprid and Diflubenzuron [3]. Therefore, in this study, the insecticidal potential of extracts from *Cycas* leaf has been explored. It is widely known for its diverse biological properties, including carcinogenic, mutagenic, neurotoxic, and teratogenic effects[4]. *Cycas* leaves contain key compounds like macrozamin and cycasin, which are toxic and of particular interest for their pesticidal activity [5]. The leaf extracts were prepared using different solvents to assess their efficacy against *Nilaparvata lugens*. We hav evaluated the insecticidal activity of different plant extracts using bioassays against this pest and achieved a mortality rate of about 83% in case of methanol fractions. Furthermore, Gas and Liquid Chromatography Mass Spectrometry (GC-MS & LC-MS) revealed the identification of the major phytochemical constituents in the extracts. The detailed methodology and results will be discussed at the conference.

Keywords: *Nilaparvata lugens,* Natural pesticides*, Cycas* leaf extract, Rice pest control

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P-52

Unprecedented Enhancement of Proton Conductivity in Metal-organic frameworks through Structural Modulation

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Proton exchange membrane fuel cells (PEMFCs) are recognized as clean energy solutions, driving the need for materials with high proton conductivity that remain stable at elevated temperatures. Nafion, the commercially dominant sulfonated fluoropolymer, demonstrates high proton conductivity (~10^{-2} S/cm), but experiences significant conductivity loss at temperatures above 80–85 °C under anhydrous conditions. Further, its amorphous structure complicates the understanding of underlying proton conduction mechanisms, hindering efforts for modification and optimization. To overcome these challenges, research is focused on developing crystalline materials with a high density of proton donor and acceptor sites to establish hydrogen-bonded networks, facilitating proton conduction. One promising class of materials that meets these requirements is metal-organic frameworks (MOFs), which are characterized by tunable structures with high micropore surface areas. In recent years, MOFs have gained significant attention for their proton conduction properties.

In our study, we examined how the proton conductivity of few stable MOFs is influenced by changes in the synthetic conditions, activation methods and modification of the MOF framework through post linker insertion. These approaches significantly enhance the proton mobility, resulting in unprecedented improvements in proton conductivity.

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P-53

Hydrogenolysis of Polyethylene by Metal-Organic Framework Confined Single-Site Ruthenium Catalysts

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Upcycling polyolefins into value-added hydrocarbons via catalytic hydrogenolysis is challenging due to poor product selectivity, random C–C bond cleavage and the formation of volatile alkanes. We have developed two isoreticular porous aluminium metal-organic frameworks (MOFs) node-supported mononuclear ruthenium dihydrides catalysts (DUT-5-RuH_2 and MIL-53-RuH_2), which are efficient in the hydrogenolysis of low-density polyethylene (LDPE) at 200 ºC into a narrow distribution of liquid hydrocarbons (C8-C24). By systematically tuning the pore sizes of the MOFs, high yields of desirable liquid alkanes were achieved with varying degrees of branching, achieving 80% selectivity. DUT-5-RuH_2 produced a C22 centred bell-shaped alkane distribution with a polyethylene conversion of 98%, while MIL-53-RuH_2, being selective for shorter alkanes, produced a C9-centred bell-shaped alkane distribution. Based on our spectroscopic and theoretical studies, the high catalytic activity and selectivity of these MOF-catalysts are primarily attributed to the stabilization of single-site mono-RuH_2 species at the MOF's nodes via active-site isolation and the confinement of the active catalytic species within porous MOFs. Theoretical calculations suggest that RuH_2-mediated polyolefin C–C bond cleavage primarily occurs via turn over limiting σ-bond metathesis. This study underscores the significance of MOFs in rationally designing heterogeneous catalysts for the efficient upcycling of plastic waste.

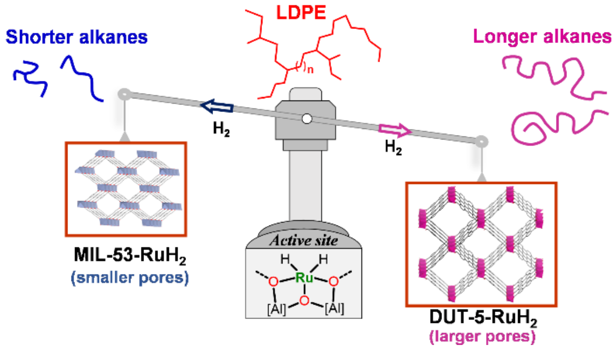

Figure 1. Graphical abstract of hydrogenolysis of polyethylene by metal-organic framework confined single-site ruthenium catalysts.

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P-54

Selective and naked eye colorimetric detection of creatinine by aptamer-based target induced passivation of gold nanoparticles

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We present a straightforward naked-eye colorimetric detection assay for creatinine, a small molecule, using gold nanoparticles (AuNPs) surface-passivated by conjugation with a creatinine-binding aptamer. The specific interaction between creatinine and the aptamer sequences reduces the catalytic activity of the AuNPs for the reduction reaction of 4-nitrophenol. Here, the surfaces of AuNPs are acted as the catalyst for the reduction of 4-nitrophenol (yellow) to 4-aminophenol (colorless) and the passivation with creatinine bound aptamer sequences delayed the reduction. This delay in colour change during the reduction of 4-nitrophenol, is employed for the quantitative detection of creatinine. The developed assay was able to detect creatinine in a linear range of 2 to 20 mM with a limit of detection of 0.87 mM. The developed colorimetric assay was very selective, reproducible and could detect creatinine in the presence of interfering biomolecules. Thae developed assay also showed excellent results for the analysis of creatinine in artificial urine samples and it can be used as point of care (POC) devices for the naked eye detection of creatinine within few minutes without any support from instruments.

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P-55

Amine-based Sequence-Defined/Conventional Polymer: Design, Synthesis, and Applications in Material and Biomedical Sciences

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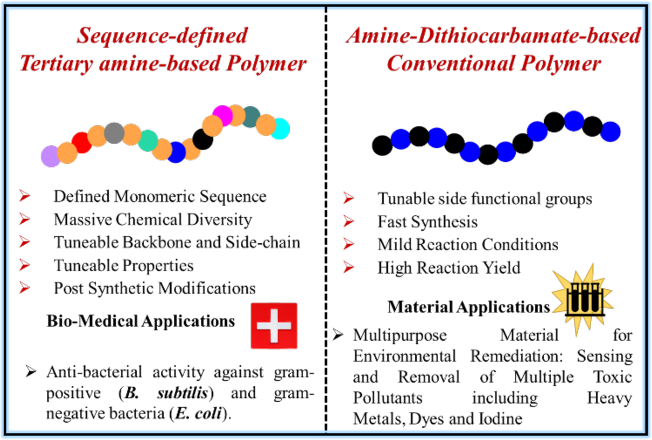
Developing macromolecules that are structurally and functionally adjustable is still challenging, even though tunable macromolecules are essential for many applications. This motivated us to focus on engineering and developing macromolecules with tuneable functional groups over the polymeric chain for diverse applications. Sequence-defined polymer (SDP) is a unique macromolecule where the polymer has perfectly defined monomer sequences and chain length. Examples include peptides, protein and oligonucleotides. Control over the monomer sequence is the key to biological activities and it is inevitable for the essential features of life [1]. Polymeric amines have gained attention recently due to diverse applications as pharmaceutical intermediates, drug/gene delivery agents, antibacterial drug, emulsifiers, cation exchange resins and catalysts. Motivated by the importance of polymeric amine compounds and sequence-defined polymer, an effort was made for the design and synthesis of a novel class of SDP by incorporating tertiary amines into the backbone from commercially available inexpensive materials. The strategy that was designed here is extremely efficient and economical for the scalable synthesis of the SDP via a support-free, protection–deprotection chemistry-free, and catalyst/template-free way. Most importantly, no extra design and synthesis of the monomer is required here [2]. After the synthesis, the biomedical applications, including the antibacterial activity of TA-SDO, were investigated against gram-positive (***B. subtilis***) and gram-negative bacteria (***E. coli***). The SDOs showed promising activity against these bacteria, and the activity of the molecules can be enhanced based on the sequences and side functional groups. These results underscore the significance of the sequences for practical applications. On the other hand, conventional polymers are simple to make, inexpensive, and less laborious. Similar to amine compounds, the dithiocarbamate (DTC) functional group possesses diverse applications in materials science and biomedical sciences. Inspired by the significance of tunable conventional polymers, DTC, and amine functional groups, we have developed a novel class of amine-DTC-based organic polymers. After synthesis and characterization, the polymers were utilised for sensing and removal of multiple harmful heavy metal contaminants, capturing radioactive iodine from water and vapor, and removal of dyes from contaminated water. In summary, an effort was undertaken to design and synthesize functionally tunable macromolecules and explore their numerous applications in the domains of materials and biomedical sciences.



- Defined Monomeric Sequence
- Massive Chemical Diversity
- Tuneable Backbone and Side-chain
- Tuneable Properties
- Post Synthetic Modifications

- Anti-bacterial activity against gram-positive (***B. subtilis***) and gram-negative bacteria (***E. coli***).

- Tunable side functional groups
- Fast Synthesis
- Mild Reaction Conditions
- High Reaction Yield

- Multipurpose Material for Environmental Remediation: Sensing and Removal of Multiple Toxic Pollutants including Heavy Metals, Dyes and Iodine

Figure 1. Graphical abstract of the Sequence-defined and Conventional polymer and their various applications.

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P-56

Cobalt isoporphyrins: Synthesis, characterization, theoretical insight and antioxidant activity

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Only zinc, iron, and copper complexes of isoporphyrin, the tautomer of porphyrin have been reported.[1] We synthesized two novel cobalt isoporphyrins: chloro[5-(methoxy)-5,10,15,20-tetrakis(4-methoxy)-5,21H-porphinato]cobalt(III) nitrate (**1b**) and chloro[5-(methoxy)-5,10,15,20-tetrakis(4-chloro)-5,21H-porphinato]cobalt(III) nitrate (**2b**). These compounds were prepared from *meso*-tetrakis(4-methoxyphenyl)porphyrincobalt(III)chloride, [Co^{III}(4-OMeTPP)Cl] (**1a**) and *meso*-tetrakis(4-chlorophenyl)porphyrincobalt(III)chloride, [Co^{III}(4-ClTPP)Cl] (**2a**) using ceric ammonium nitrate (CAN) in methanol as the oxidizing agent.[2-3] We characterized the compounds using UV-Visible, mass spectrometry (ESI), FTIR, and ^{1}H NMR spectroscopy. The methoxy cobalt isoporphyrins exhibit significant instability, as revealed by electrochemical studies. In this presentation, we will review our efforts to understand the distinct properties of these cobalt methoxy isoporphyrins, including theoretical investigations at the DFT level, which include geometry optimization, energy calculations, UV-Vis spectral simulations, NBO analysis, and global reactivity indices.

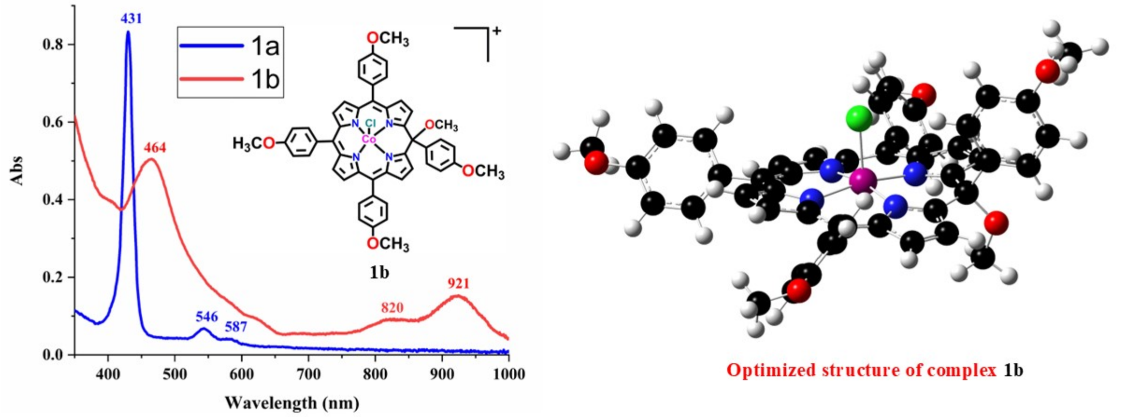

Figure 1. Graphical abstract of the cobalt methoxy isoporphyrins.

NBO investigations indicate that intramolecular charge transfer occurs within the synthesized complex. The global reactivity indices further confirm the reactive nature of cobalt isoporphyrins in comparison to Fe and Zn-methoxy isoporphyrins.[4] Additionally, we examined the antioxidant properties of cobalt methoxy isoporphyrins and compared them to their parent porphyrins, finding that complex **1b** exhibits the highest antioxidant activity of 82%.

Keywords: Isoporphhyrin, Cobalt (III) porphyrin, Density Functional Theory, Antioxidant activity, Global reactivity indices.

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P-57

Controlled modulation of nanometric roughness and surface free energy with rewritable liquid selective patterns

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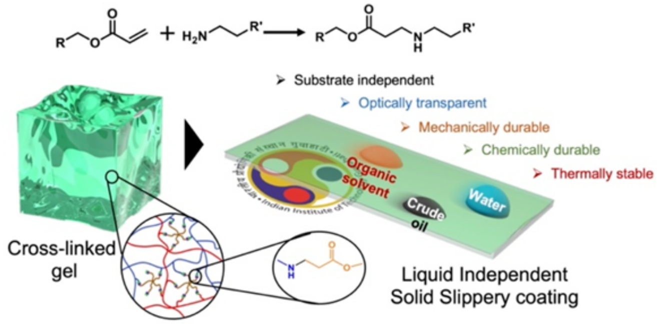
Smooth interfaces with low surface free energy enable effortless sliding of liquid droplets with homogeneous wettability, displaying low to moderate contact angles, unlike superhydrophobic interfaces [1]. These slippery surfaces are promising alternatives to extremely liquid-repellent, hierarchically rough interfaces, which suffer from instability under severe conditions, light scattering, and entrapment of fine particles [2]. However, designing a solid, dry antifouling interface requires precise modulation of surface free energy and nanometric roughness. We demonstrate the use of covalent cross-linking chemistry to modulate surface free energy (from ~49 mN m^{-1} to ~22 mN m^{-1}) and roughness (root mean square roughness from 30 nm to 3 nm) for robust, liquid- and substrate-independent slippery properties. By strategically selecting a β-amino-ester linkage through a 1,4-conjugated addition reaction between amine and acrylate groups in a three-component reaction mixture under ambient conditions, we achieved self-cleaning ability, anti-smudge properties against both water and oil-based inks, thermal stability (>300 °C), chemical stability, physical durability, and optical transparency (~95%). The slippery properties of the coating remained unaffected at elevated temperatures making it suitable for maintaining the performance of solar cell modules and other objects under outdoor conditions [3]. Taking the advantage of SFE and roughness, we additionally introduced a 'liquid-specific' wettability pattern through selectively sacrificing the slippery property against only low γ_{LV} (<30 mN m^{-1}) liquids where the design included a chemically reactive crystalline network of phase-transitioning polymer, which displays an effortless sliding of both low and high γ_{LV} liquids [4]. With these, we have made a 'rewritable' and 'liquid-specific' wettability pattern for high throughput screening, separating, and remoulding non-aqueous liquids.



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P-58

Self-Consistent-Field Solution for Unstable Anions

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When using a diffuse basis set to study unstable or temporary anions, the SCF solution often collapses into a minimum energy solution with an extra electron in the most diffuse MO present in the basis set. If more diffuse functions are added to the basis set, the SCF solution for the corresponding unstable anion ultimately converges into a neutral molecule and a free electron. This is known as variational collapse. Therefore, the SCF solution should not be trusted for further use.

The modified PEM is implemented in conjunction with the nuclear charge stabilization method to obtain a meaningful SCF solution for an unstable anion with an extra electron in the valence framework rather than being present in the diffuse MO. The obtained SCF solution, which avoids the variational collapse, may now be used in post-SCF calculation to account for electron correlation.

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P-59

Design, Synthesis and Structural analysis of Indole-linked 1,3,4-Oxadiazole Thioglycosides as potential Antibacterial agents

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Keyword: Indole, thioglycoside, 1,3,4-oxadiazole, antibacterial

Many five-membered, six-membered, and fused heterocycles have potential biological properties such as antibacterial, antifungal, antitumor, antioxidant, anti-inflammatory etc.[1] Indole and oxadiazole motif hybrids are effective against multidrug-resistant bacterial microorganisms.[2] The presence of carbohydrates (polyhydroxy groups) in hybrids enhances the water solubility and reduces the toxicity. This property helps in a more effective drug development process.[3] Consequently, we designed and synthesised novel Indole based S-alkylated/ S-arylated and S-glycosylated 1,3,4-Oxadiazole derivatives. Structural confirmation of all the compounds were done on the basis of spectroscopic techniques including ^{1}H, ^{13}C NMR, FT-IR, HRMS, and XRD data. The antibacterial potency of target compounds was further evaluated against various gram-positive and gram-negative bacteria.

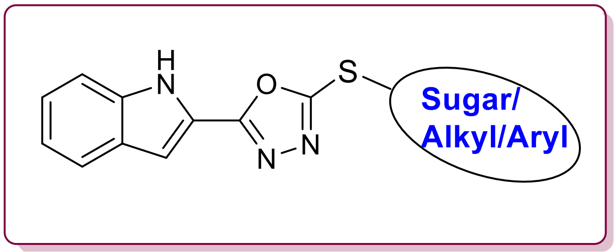

Fig- 1. Synthesis of Indole 2-(1,3,4-oxadiazolyl) S-alkyl/S-aryl/S-sugar derivatives

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P-60

An ab Initio Study on the Photoisomerization in 2-styrylpyridine

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The intersection of photochemistry and material science has given rise to a promising avenue of research, wherein the controlled manipulation of molecular structures plays an important role in unlocking unprecedented functionalities in materials. This led the development and application of photochromic molecular switches (molecular photoswitches) and molecular memories to become one of the most active fields of research.[1][2] Photochromic materials like diarylethene,[1] azobenzen[3] and stilbene[4] are well-suited candidates for photoswitches and photomemories due to their unique combination of reversibility, tunability, fast response times and stability. Irradiation of photochromic materials leads to isomerization or color changes which are accompanied by reversible changes in their geometrical structure, quantum yield and absorption spectra between the different states.[5] This controlled switching enables the selective activation and deactivation for photoswitches[2] and tailored responses in photomemories.[6] Such applications have instigated further investigation into photoisomerization processes in vinylene- and azo-linked compounds for improved responsiveness, tunable functionalities and stability, which are fundamental to unlock new possibilities for developing innovative materials with potentially enhanced electro-optical properties. The photoinduced isomerization of the Styrylpyridine(STPY) derivative incorporated in transition metal complexes has been shown to be a means of enabling photocontrol of the switching and reactivity of these complexes.[7] This has piqued our interest to carry out characterization of the photoactive STPY molecule.

To the best of our knowledge, the photoisomerization and photocyclization of 2-STPY, along with their possible relaxation pathways has not yet been explored. Therefore in this presentation, we are going to report on the theoretical study on photoinduced isomerization in 2-STPY. Firstly, the geometries and the relative energies of the possible conformers were investigated within second-order Møller-Plesset (MP2) and algebraic diagrammatic construction to second-order (ADC(2)) theories with the cc-pVTZ basis set. The complete active space self consistent field (CASSCF) method is used for locating the S1/S0 minimum energy conical intersection (MECI) structures. In addition to the twisted-pyramidalized MECI points along the trans and cis isomerization pathways, S1\S0 cooperating-ring MECI and cyclized-ring MECI structures, lying on the cyclization pathways of cis 2-STPY were also located. We have identified the MECI points which are found to be accessible from either one or more Franck-Condon points. The possibilities for the cis–trans isomerization and cyclization processes are discussed along the image-dependent pair potential paths(IDPP).

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P-61

Harnessing Fluid Dynamics Using Photoresponsive Materials for Advanced Spatiotemporal Patterning

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Spatiotemporal patterning driven by biological molecules is the key to understanding the emergence of ordered structures in living organisms. Thus, it is important to understand the local interactions of these collective behaviors. However, creating spatiotemporal patterns in synthetic system is very challenging. Herein, we designed a liquid crystal-based light-actuated micropumps consisting of azobenzene moiety that turns on fluid flow upon UV light illumination via isomerization of trans-azobenzene to cis-azobenzene. The fluid flow direction was reversed when UV light was turned off. Interestingly, the azobenzene-based film alone could not produce directional motion under UV exposure. However, the flow was amplified to many folds in the presence of liquid crystal matrix. The intrinsic contractile and expanding nature of liquid crystal in the presence of photo-responsive azobenzene triggered the fluid flow. Later, the photo-isomerism of azobenzene was utilized to create a flow oscillation that eventually led to spatiotemporal patterning of colloids. Chemical-free on-demand flow reversal and spatiotemporal patterning are the unique features of the current systems. This technology has the potential to be integrated with a microfluidic device that can employ liquid crystal film to regulate the fluid flow direction.

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P-62

Lignin nanocomposite films: Advanced UV protective and antimicrobial sustainable materials

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Lignin, a renewable aromatic biopolymer, holds significant potential for applications in bio-refineries, biofuels, thermoplastics, and eco-friendly nanofilms. Transforming lignin-based biomass into biodegradable nanofilms is vital. India's nanofilm exports are limited, largely relying on costly imported nanomaterials. Utilizing the alkaline extraction method, utilizing diverse base concentrations and reaction temperatures, yields high lignin output with lower chemical and energy input, suitable for large-scale production. Converting lignin to nano size and utilizing it as self-cleaning and UV protective nanofilms, enhances properties from mechanical strength to antibacterial and antioxidant functions. Lignin-doped polyvinyl alcohol/polyethylene glycol nanocomposites exhibit increased flexibility and strength. Lignin nanofilms showcase paralleling commercial counterparts, suggesting potential for eco-friendly coatings and insulation. These nanofilms unite cost-effectiveness, agri-waste sourced lignin, and multi-functionality. Lignin-derived nanoparticles are synthesized from agricultural waste, bypassing harmful chemicals, yielding affordable nanofilms. The innovation simultaneously repurposes agricultural waste into lignin-based, multi-functional nanofilms, offering self-cleaning, and cost efficiency in a single sustainable product.

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Indian Patent Appl. 202211070754

Seema Kirar, Devesh Mohne, Manali Singh, Varsha Sagar, Anil Bhise, Saswata Goswami, Jayeeta Bhaumik, Eco-friendly lignin nanocomposite films as advanced UV protective and antimicrobial sustainable packaging materials, Sustainable Materials and Technologies, Volume 40, 2024, e00864, ISSN 2214-9937, https://doi.org/10.1016/j.susmat.2024.e00864.

P-63

Stable and Reliable Synthesis of Graphene Oxide via the Tour's Method

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Graphene oxide (GO) has garnered significant attention for its diverse applications in energy storage, environmental remediation, and sensor technology. GO is the oxidation form of Graphene. The present study aims to optimize the GO synthesis elucidates via Tour's method, which enhances the oxidation of graphite using sulfuric acid and potassium permanganate. This approach yields high-quality GO with minimal impurities, improves the oxidation process, eases temperature control, and does not release toxic gases. UV-Vis, XRD, FTIR, and SEM validate the superior properties of the synthesized GO. The advantages of the Tour's method position it as an optimal choice for the scalable production of graphene oxide, facilitating its application across various fields.

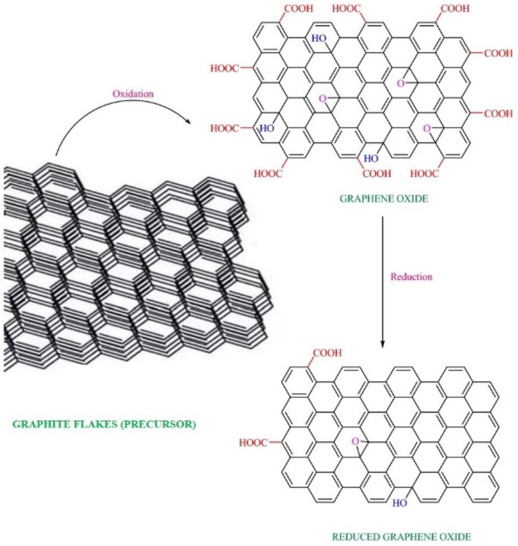

Figure 1. Synthesis route of graphene oxide and reduced graphene oxide [1].

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P-64

Stable *peri*-Naphthoisatogens without C2 Protection: Synthesis via Aldrone Condensation, Optical Properties and1,3-Dipolar Cycloaddition Reaction

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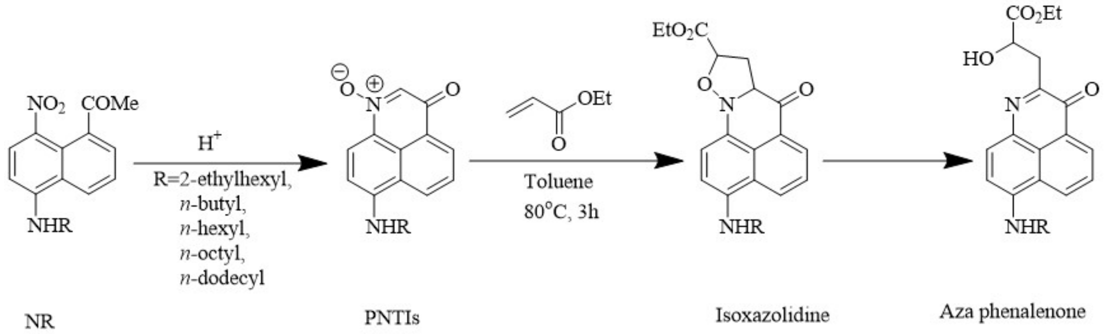
Annulating naphthalene with functional groups through peri-positions allows for the creation of diverse molecules with unique characteristics and applications. For example, They are widely used in several fields such as sensors, pharmaceutical chemistry, supramolecular chemistry, and materials chemistry. In spite of their wide range utilities, naphthalene derivatives have restricted functional groups such as imides, amides, and diamino derivatives (perimidines). Therefore, *p*eri-annulation should be done with novel functional groups to improve the diversity of naphthalene derivatives. We took up the challenge to make a contribution in this underdeveloped field, and herein report on the synthesis, derivatization, and optical characteristics of five novel *peri*-naphthoisatogens (PNTIs) dyes via incorporation of α-keto aldonitrone as a new functional group. The synthesis was carried out via an uncommon aromatic nitro group reaction, which involved the nucleophilic attack of a C-nucleophile (enol) on the N-atom of the nitro group. In five distinct 5-alkylamino-8-nitro-1-acetylnaphthalenes (NR), intra-molecular acid-mediated nucleophilic attack of the enol moiety on the N-atom of the nitro group generated α-keto aldonitrone via addition-elimination process. The PNTIs exhibited 1,3-dipole properties and reacted with ethyl acrylate to form an isoxazolidine ring, which was then transformed into an aza-phenalenone derivative via ring cleavage.. Both the PNTI and the corresponding derivative strongly absorb in the visible region, displaying absorption maximum at 551 and 561 nm (in CHCl3) respectively. Compared to the popular analogous dye naphthalene monoimides, PNTIs showed bathochromic shift of absorption maximum by more than 100 nm. The emission maximum for the PNTI and its derivative in chloroform were observed at 594 and 635 nm respectively.



Scheme 1: Synthesis of PNTIs via Aldrone condensation reaction and subsequent 1,3-Dipolar Cycloaddition reaction of PNTIs

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P-65

Heterotopic Cooperativity in Human CYP3A4 Mediated by Multi-Drug Interactions

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Molecular recognition is a fundamental process in all biological systems and is of significant interest in structure-based drug design. To date, 50 human P450 variants have been identified, with CYP3A4 standing out as a major drug-metabolizing enzyme due to its remarkable substrate promiscuity. CYP3A4 is known to bind multiple copies of various compounds, oftendisplaying cooperative behavior in the presence of multiple substrates. This multi-drug interaction can sometimes result in inhibition of CYP3A4-mediated metabolism, making the study of heterotopic cooperativity, facilitated by multiple ligands, an important yet underexplored area.

In this study, we aimed to investigate heterotopic cooperativity and atypical kinetics in monomeric CYP3A4 using three drugs: the sedative midazolam (MDZ), the anticonvulsant carbamazepine (CBZ), and progesterone (PGS). We conducted extensive unbiased moleculardynamics simulations, supported by adaptive sampling methods guided by Markov state models, resulting in approximately 60 µs of total sampling with CYP3A4 in complex with each substrate. To further probe the cooperative mechanisms, we designed and executed a series of metadynamics simulations across several conformations.

Our findings reveal the cooperativity of MDZ, CBZ, and PGS in multi-drug scenarios, and weidentified key metastable states and molecular hotspots that provide mechanistic insight into heterotopic cooperativity and atypical kinetics. This study offers a deeper understanding of CYP3A4's function in the presence of multiple drugs.

This research was supported by the high-performance computing facilities at the Tata Institute of Fundamental Research, Hyderabad, and the Department of Atomic Energy Commission, Government of India.

P-66

Synthesis of Starch-PANI as biosorbent to remove methyl blue from water and study its antioxidant and electrochemical properties

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In the recent years, there has been considerable interest in the synthesis of biopolymer based polymer composites. This becomes an important area of composite research because of its application in material science[1] and also due to its chemical structure, biocompatibility, and biodegradability[2]. In this work, we have synthesized Starch-PANI composite and studied their adsorptive performance and electrochemical properties.

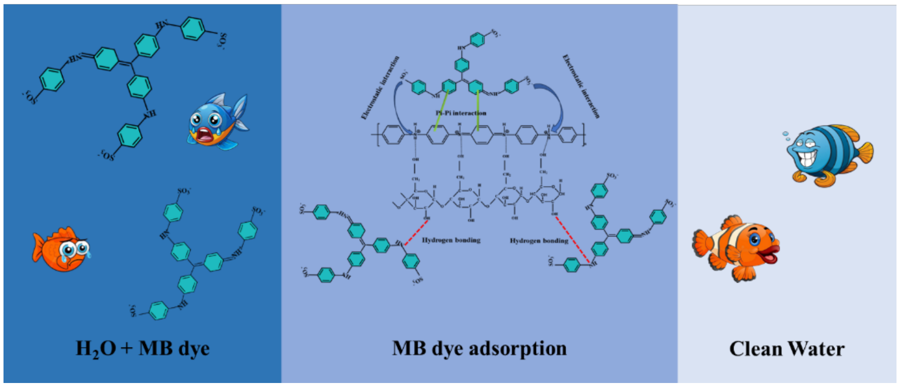

Figure 1. Graphical abstract of Starch-PANI biosorbent to remove MB dye from waste water

These materials were prepared and characterised with FTIR, XRD, SEM, UV and TGA analysis and further evaluated for their methyl blue (MB) dye adsorption characteristics from aqueous solution. The effects of initial dye concentration, contact time, pH and adsorbent concentration on the adsorption capacity of Starch-PANI for MB have been studied. The adsorption kinetics and isotherm of MB by Starch-PANI were studied. Its maximum adsorption capacity was found to be 13.97429 mg g^{-1}. The adsorption of MB dye molecules by Starch-PANI followed pseudo-second-order kinetic model and Langmuir isotherm, and it was a spontaneous, monolayer and chemical adsorption process. Moreover, we have studied the antioxidant and different electrochemical properties of the synthesized composite.

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P-67

Synthesis, Characterization and Application of an Acid Modified Biochar: A potential Adsorbent for the Malachite green

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Biochar, derived from waste biomass that includes Lagenaria siceraria seeds, is an accessible and non-toxic material that has garnered significant interest as a potential solution for the elimination of water contaminants. The introduction of phosphoric acid as an activator in a 1:2 ratio for biochar modification offers a viable method to improve the adsorption capacity for malachite green dye. [1] Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), X-ray diffraction (XRD), and surface area (BET) were the techniques that were utilized in order to define the characteristics of both the phosphoric acid-treated and untreated biochar. Based on the findings of Fourier transform infrared spectroscopy, the phosphorus-containing functional groups of modified biochar, such as P=O and P=OOH, interacted with dye and also formed complexes with it. This interaction likely has led to the improved adsorption of malachite green dye compared to pure biochar. [2] The studies on the adsorption mechanism observed multiple interactions taking part in the adsorption process, including electrostatic interactions, hydrogen bonding, π-π interactions, pore filling. [3] The study examined the removal efficiencies of dye under varying pH levels, time durations, concentrations of pollutants, and adsorbent dosages, achieving a 99.5% removal efficiency in less than one hour. According to the findings, the phosphoric treatment improves the physicochemical features of the biochar by means of a bigger surface area and enrichment of oxygen-containing functional groups in comparison to the biochar that are in their natural state.

Keywords: Acid modified biochar, Adsorption, Malachite green.

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P-68

External and internal stimuli for enhanced supercapacitor performance

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Supercapacitors, also known as electrochemical capacitors, are energy storage devices that bridge the gap between conventional capacitors and batteries.[1] They exhibit high power density, fast charge/discharge rates, and long cycle life, making them suitable for various applications, including electric vehicles, portable electronics, and grid energy storage. Supercapacitors store energy through electrostatic charge accumulation or faradaic processes at the electrode-electrolyte interface. The performance of supercapacitors is influenced by factors such as electrode material, electrolyte composition, and device architecture.[2] This presentation highlights how both internal and external factors impact the material fabrication and electrochemical performance of supercapacitors, while also exploring the mechanisms of energy storage within these devices.

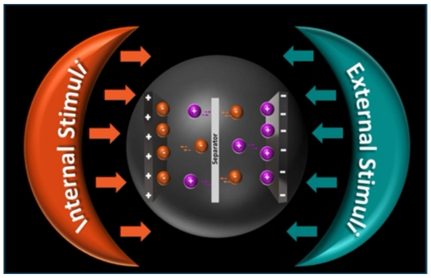

Figure 1. Illustration of the impact of internal and external stimuli on the energy storage mechanism of a supercapacitor

The use of internal and external stimuli offers an alternative approach to overcoming the limitations of supercapacitors, enhancing their electrochemical properties. Internal stimuli, such as redox-active dopants and vacancies, can modify the electronic structure or phase of electrode materials, improving redox behavior in pseudo-capacitors through electron polarization, which enhances electrochemical charge transfer kinetics. Conversely, external stimuli, such as an applied magnetic field, can affect the diffusion characteristics of active ions in the electrolyte, altering ion rearrangement and diffusion within the supercapacitor electrodes.[3] This interaction between magnetic fields and electrode materials leads to the development of magneto-supercapacitance. Future research in this interdisciplinary area presents promising opportunities to improve energy storage technologies and overcome existing challenges.

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P-69

Electron-donor-acceptor (EDA) complex-driven regioselective vicinal and oxidative geminal functionalization of alkynes†

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A visible-light-initiated electron-donor-acceptor (EDA) complex-driven regioselective vicinal and oxidative geminal thiosulfonylation of alkynes is presented. Organic thiosulfonates act as an acceptor, producing either sulfonyl ($RSO_2^{\bullet}$) or thiyl ($RS^{\bullet}$) radicals under base and solvent switchable conditions. Simultaneous installation of three different functionalities, *viz* carbonyl, sulfonyl, and thiyl, takes place under one condition, while another condition leads to vicinal thiolation and sulfonylation.

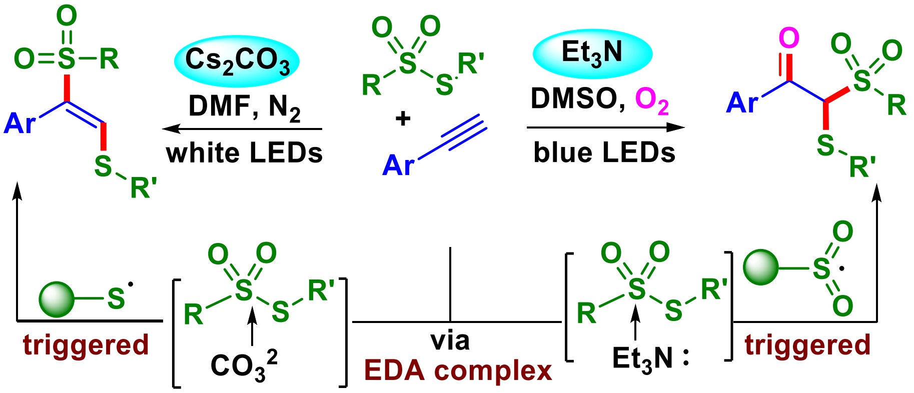

Figure 1. Electron-donor-acceptor (EDA) complex-driven regioselective vicinal and oxidative geminal functionalization of alkynes†

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[1] Chem. Commun., 2024, ASAP, DOI 10.1039/D4CC04610B

P-70

Oxidative Carbotrifluoromethylation of Maleimides with Imidazopyridines and Langlois' Reagent Mediated by PIDA

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An unprecedented methodology for oxidative carbotrifluoromethylation of maleimides with imidazopyridines and Langlois' reagent as coupling partners has been developed to afford 3,4-disubstituted maleimides employing (diacetoxyiodo)benzene (PIDA) as an oxidant. Introduction of trifluoromethyl ($-CF_3$) group in any organic moiety always enhance the significance of the molecule pharmaceutically.[1] Additionally, among *N*-containing heterocycles, imidazopyridine is important for its wide application in several marketed drugs.[2] Maleimides also has several applications in natural products.[3] The present method demonstrates installation of two biologically important moieties: imidazopyridine and trifluoromethyl group across the double bond of maleimides under metal-free conditions.[4] Both experimental and theoretical studies support the proposed radical reaction mechanism.

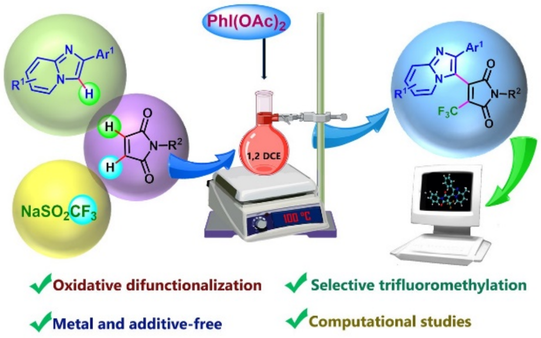

Figure 1: Oxidative Carbotrifluoromethylation of Maleimides with Imidazopyridines and Langlois' Reagent

The optimized reaction conditions for the current protocol were achieved after investigation of the requisite conditions. The scope of the reaction was further explored with variation of coupling partners: imidazopyridines and maleimides. The reaction was well compatible with a variety of substrates. A series of control experiments were performed to depict the mechanistic pathway for the reaction and GC-MS analysis was done to show the generation of trifluoromethyl radical in the reaction medium. A plausible mechanistic pathway based on control experiments and literature study was demonstrated. DFT study was performed to support the proposed mechanistic pathway.

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P-71

A Chiral Photo Switchable Cage

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The ability of hollow imine-based cages to accommodate small guests inside their central cavity can be made more valuable and widely applicable if the host-guest interactions can be controllably modulated, allowing for reversible guest uptake/release in response an external stimulus[1]. Such stimuli may include chemical, electrochemical, or photochemical signals, with light being particularly advantageous due to its precise tunability in wavelength and intensity, cleanliness, and ease of delivery.[2] Azo-based cages, however, often face a limitation in achieving high photoisomerization efficiency, restricting their broader practical applications.[3] Addressing this challenge, we present a chiral photoswitchable cage that improves photoisomerization efficiency while enhancing chiroptical properties.

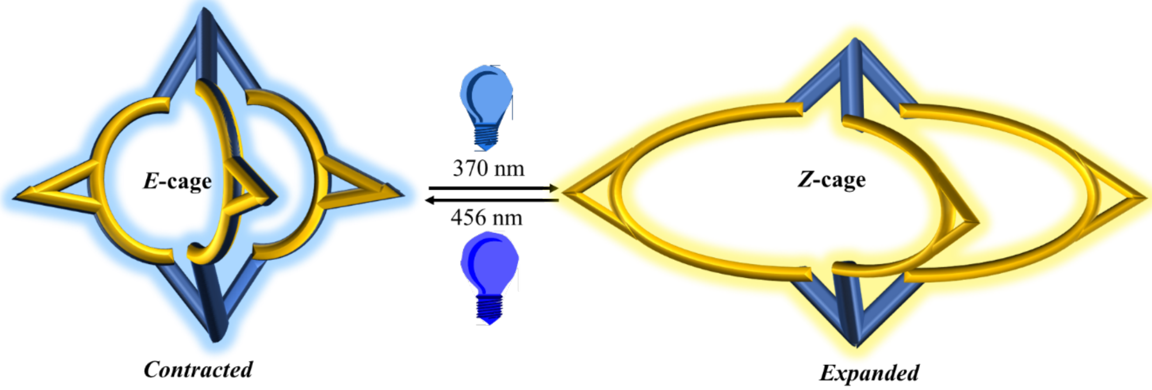

Figure 1. Cartoon representation of the switching between contracted and expanded cage

In this work azobenzene is taken as the switchable unit which is embedded with a chiral BINOL aldehyde through flexible spacer. In order to make cage, the three aldehyde ligands were combined with two tris(2-aminoethyl)amine molecules, resulting in six imine bonds. The chiroptical properties of this chiral cage was investigated through CD spectroscopy. The photoswitching experiments revealed intriguing results. When irradiated at 370 nm, the cage underwent structural changes in both the overall framework and the azobenzene units while maintaining its composition. The photoisomerization efficiency of the cage is twofold greater compared to the aldehyde ligand as the cage structure distorts the plane of *E*-azo units. Additionally, the CD spectra showed changes which relates to the overall structural changes of the cage. This suggests that the cage cavity can be suitable for the selective uptake and release of chiral guests.

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P-72

Synthesis and characterization of Eco-friendly biolubricant from *Brassica carinata* oil: Parameter optimizations using Response surface methodology

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This research highlights the potential of the *Brassica carinata* as a sustainable substitute in the lubricant industry by examining its viability and effectiveness in producing biolubricants. In the present work, the biolubricant was synthesized via a double transesterification method. Initially, *Brassica carinata* oil undergoes transesterification with KOH and methanol to yield FAMEs. Subsequently, these FAMEs react with 2-ethyl hexanol using p-TSA as a catalyst to produce *Brassica carinata*-based ethyl hexyl ester. The central composite design of the experiment was chosen to optimize and examine the effects of production variables, such as temperature, FAME-to-2-ethyl hexanol molar ratio, and catalyst concentration. The optimum bio-lubricant yield of 84.3 % was achieved using a FAME-to-2-ethyl hexanol molar ratio of 1:3, a reaction temperature of 110°C, and a catalyst concentration of 5wt%. The predicted yield agreed with the experimental value, with $R^2 = 0.9785$, which signifies a strong relationship between the independent and dependent variables. Further, GC-FID analysis, NMR spectroscopy, and FT-IR spectroscopy of the synthesized product confirm its successful synthesis. Finally, the significant physicochemical properties of the product, such as density at 15 ºC, pour point, coefficient of friction and wear scar diameter, were found to be 0.8736 g/cm3, -30°C, 0.06, and 0.862 mm, respectively.

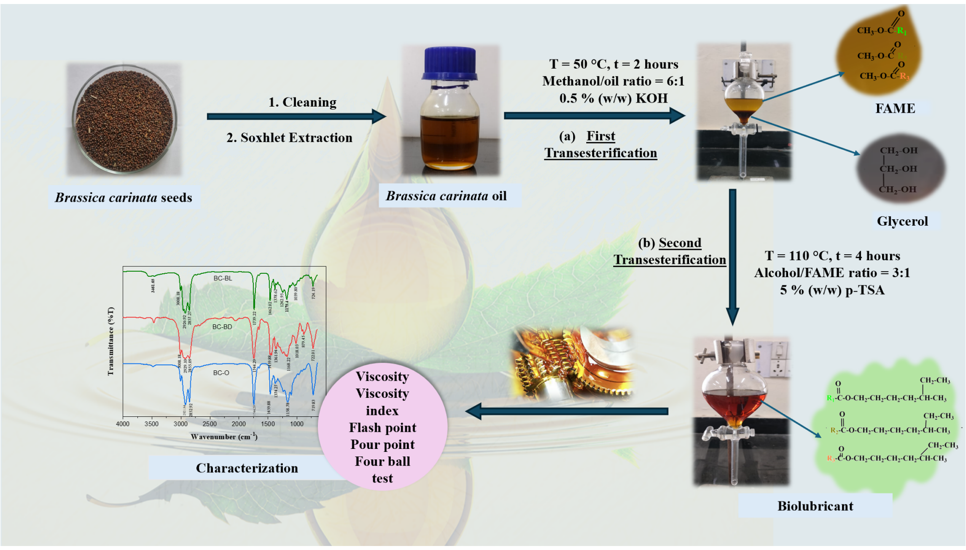

Figure 1. Graphical abstract of the biolubricant synthesis from *Brassica carinata* oil

P-73

Spirobifluorene-BINOL based Polymer Nanoreactor Harnessing Efficient Synthesis of 1*H*-Tetrazole and Iodine Adsorption with Facile Charge Transfer

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Multifunctional porous polymeric nanoreactors are visually appealing and need insightful design strategy. Our work delineates a novel method for developing the porous polymer **SBF-BINOL-6** by forming the BINOL entity in situ using spirobifluorene and naphthols as co-monomers and achieving a high yield of 81%.[1] The polymer as produced featured nanotube and nanosphere like morphology, thermal endurance reaching 372 °C, and a BET surface area of up to 590 m^2 /g. The polymer enabled the effective loading of silver nanoparticles to produce **Ag@SBF6**, as demonstrated by high resolution transmission electron microscopy and X-ray photoelectron spectroscopy. With yields ranging from 75 to 99% and recyclability for at least seven times without degradation, the **Ag@SBF6** was successfully employed as a heterogeneous catalyst towards the [3+2] dipolar cycloaddition process for the production of physiologically significant 5-substituted 1*H*-tetrazoles. Furthermore, the iodine-loaded polymer, **I_2@SBF6**, showed that iodine promoted increased conductivity (1.3×10^{-3} $S.cm^{-1}$) through simple charge transfer interactions. This was made possible by the polymer's superior host-guest interaction, which allowed for iodine adsorption in the vapour phase with a high uptake capacity up to 4.0 $g.g^{-1}$ (Figure 1).

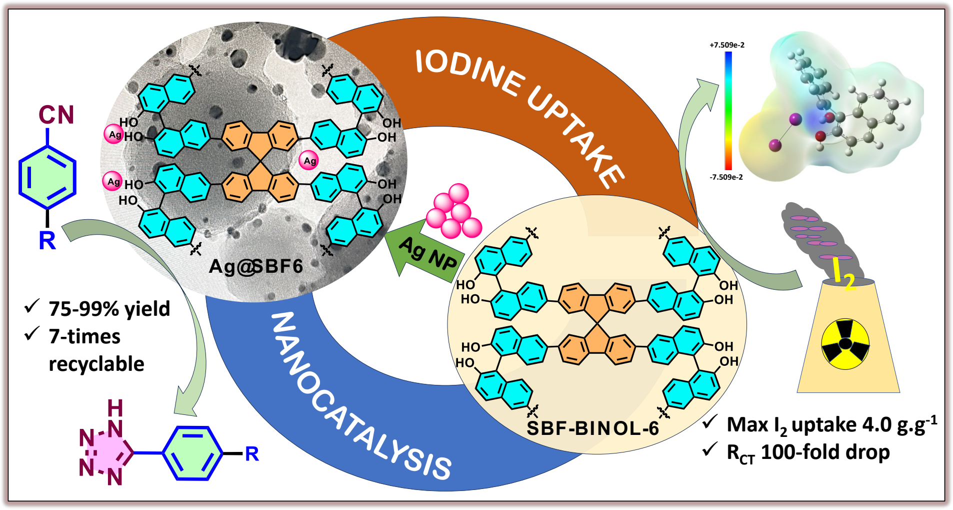

Figure 1. **SBF-BINOL-6** as multifunctional host towards iodine and Ag NPs

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P-74

Ytterbium(III)Triflate Catalyzed (3+2) Annulation of Spiro Donor-Acceptor Cyclopropanes with Thiourea: Access to Spiro Tetrahydrothiophenes

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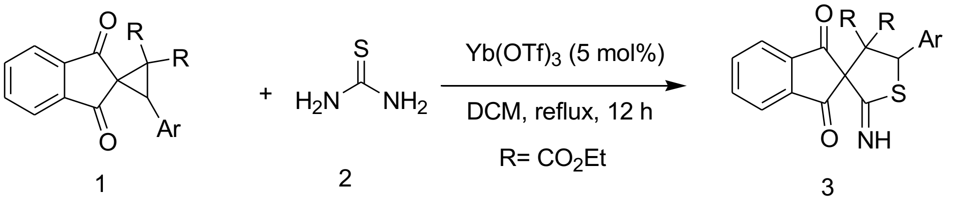
Tetrahydrothiophene ring system is widespread among various medicinally relevant natural products such as biotin, salacinol, ponkoranol and kotalanol. Due to the importance of tetrahydrothiophenes, extensive research efforts have been devoted in both industrial and academic settings for their synthesis.[1] Donor–acceptor (D–A) cyclopropanes are versatile three-carbon building blocks for the synthesis of various carbo and hetrocycles. They undergo Lewis acid mediated (3+*n*) annulation reactions with various dipolarophiles, containing C=C, C=O, C=N, N=O, N=N, C≡C, and C≡N units.[2] However the dipolarophiles having C=S unit have been rarely employed as annulation partners to react with D–A cyclopropanes. Even though such annulations have yielded tertrahydrothiophenes,[3] the synthetic utility of spiro D–A cyclopropanes **1** towards synthesis of spiro tetrahydrothiophenes remains unexplored. To fill the gap, we reacted spiro D–A cyclopropanes **1** with thiourea **2** in presence of catalytic amount of Yb(OTf)$_3$ in DCM under reflux conditions the reaction afforded highly substituted spiro tetrahydrothiophenes **3** in good yields. The details will be presented in the poster.



Scheme 1

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P-75

Energy Enhancement of a Nickel−Cobalt-Mixed Metallic Metal−Organic Framework Electrode and a Potassium Iodide Redox Mediator Bound with an Aqueous Electrolyte for High-Performance Redox-Aided Asymmetric Supercapacitors

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In recent years, increasing energy demands in industry and human science call for efficient, clean energy conversion and storage devices. Therefore, improved energy storage technologies are urgently required. Batteries and supercapacitors have emerged as promising possibilities, and they have seen a lot of use in electronic vehicles and electronic gadgets. Compared with batteries, supercapacitors exhibit a fast charge and discharge capability, high power density, and high cycle stability [1] Generally, Various materials such as metal oxides, metal organic frameworks (MOFs), covalent organic frameworks (COFs), conducting polymers (CPs), metal chalcogenides, etc., exhibits pseudocapacitance. Contemporarily, researchers have increasingly focused on Metal−organic framework (MOF) materials with redox active metal ions have improved the pore structure and have been continually exploited for energy storage because of their unique Pseudocapacitive nature.[2] By using KI redox mediator electrolyte, pseudocapacitance can increase the power density, and cycle stability is observed in the electrode material for supercapacitors.

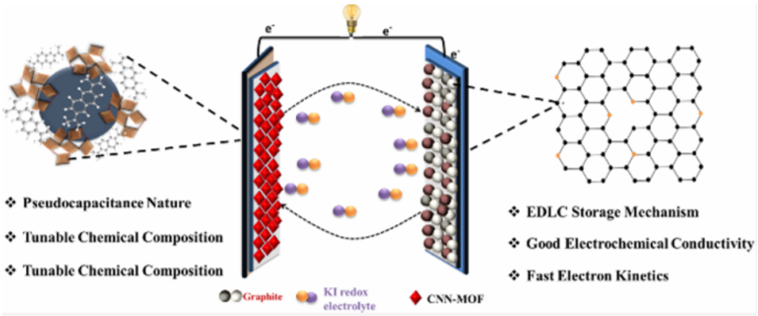

Figure 1. Graphical abstract of the fabricated RAASC device.

Enhancing the energy density of supercapacitors requires the development of novel electrode and electrolyte materials that can endure high voltages and exhibit fast electrochemical kinetics. Pseudocapacitance, high energy density, and specific capacitance can be achieved through electrodes and redox mediator electrolytes used in redox-aided asymmetric supercapacitors (RAASC), which are vital for their practical application. In this study, a rod and microsphere structure of Ni/Co-mixed metal-organic framework (MOF) was synthesized using a hydrothermal method for the positive electrode material. The rod and microsphere structure provides numerous active sites and smooth ionic channels, making Ni/Co-MOF a suitable material with three different organic linkers. The CNN-MOF material, which has a rod-like structure, demonstrated good capacitance. To further improve its capacitance, a KI redox mediator combined with a KOH electrolyte was introduced, achieving a specific capacitance of up to 612 F g^{-1} in a three-electrode system. Additionally, in the assembled RAASC, a graphite anode with CNN-MOF as the cathode and a KI redox mediator bound with a KOH gel polymer electrolyte exhibited electrical double-layer capacitor behavior. The RAASC device achieved an energy density of 84.2 W h kg^{-1} and a power density of 532 W kg^{-1}. It also displayed excellent cyclic stability, retaining 97.4% of its initial capacitance after 11,200 charge/discharge cycles. This work highlights the efficient fabrication of high-performance MOF electrodes and introduces the KI redox electrolyte-constructed RAASC device as a promising approach for advanced energy storage systems.

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P-76

Ferric Chloride Mediated Dearomative Spirocyclization of Biaryl Ynones: Synthesis of 3,3-Spiroindanones

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Indanones are privileged structural motifs widely present in many natural products and synthetically bioactive molecules.[1] Furthermore, indanone derivatives are widely used as fluorophores, dyes, organic functional materials, and OLEDs.[2] As a consequence, various metal-catalyzed or metal-free approaches have been adopted to create 1-indanone core. Similarly, the creation of spiro compounds with inherent rigidity and complexity has long been a goal for synthetic organic chemists.[3] Various approaches have been documented for building the spiroindanones framework.[4] However, only few reports are known for 3,3-spiroindnanones.[5]

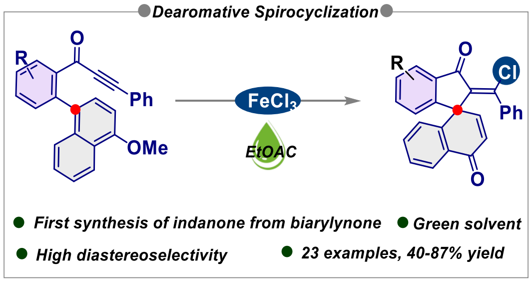

Figure 1. synthesis of 3,3-spiro-1 indanone frameworks

We have developed a dearomative spirocyclization for the synthesis of new series of densely functionalized 3,3-spiroindanone derivatives. This work reports, for the first time, the regioselective synthesis of a five-membered ring from biaryl ynones. Few synthetic application reactions have also been performed. In light of indanones, substantial therapeutic significance, the pharmaceutical industry might find our methodology valuable.

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P-77

A DFT study of H_2 Production from Water Splitting by using Bare and Transition Metal Doped Ti_2O_4 Clusters

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Fossil fuel energy is unsustainable because of its limitations, depletion, and environmental impacts. Environmental issues associated with fossil fuel-based energy systems include CO_2 and greenhouse gas emissions, air pollution, global warming, fossil fuel combustion, exhaustible and depleting energy sources, acid rain, and environmental degradation. [1] In the field of renewable energy, hydrogen (H_2) has been considered a promising energy carrier that has the potential to replace current fossil fuel-based energy sources. Hydrogen is a clean, renewable fuel that has the potential to be a future energy carrier. A large reduction in carbon emissions can be obtained by manufacturing hydrogen using renewable energy sources.[2] Green hydrogen is a clean and sustainable energy source that causes significantly lower greenhouse gas emissions. Transition metal oxides, such as zinc oxide (ZnO), titanium dioxide (TiO_2), ruthenium dioxide (RuO_2) etc., have potential applications for the water splitting reaction (WSR) process.[3] Density functional theory (DFT) method is used to investigate the formation of H_2 molecules from hydrolysis products formed by H_2O addition to metal oxide clusters. In this regard, we have performed computational study of H_2 production from water splitting by using bare and transition metal doped Ti_2O_4 clusters.

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P-78

Design, synthesis and molecular docking study of novel Triazole-Quinazolinone hybrids as antimalarial agents

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Keywords: Antimalarial, Triazole, Quinazolinone, Molecular docking

In our ongoing search toward discovering novel antimalarial drugs, we have designed and synthesized a series of novel Triazole-Quinazolinone hybrids. The in vitro screening of the Triazole–Quinazolinone hybrid entities against the Plasmodium species P.falciparum offered potent antimalarial molecules **6c**, **6d**, **6f**, **6g**, **6j**& **6k** owing comparable activity to the reference drugs. The cytotoxicity of the most active compounds was studied against the RAW 264.7 cell line by MTT assay and no toxicity was observed. A molecular docking study was conducted to explore the features of target molecules. The study indicates that all the molecules are binding to the Falcipain-2 protease (PDB: 6SSZ) of the P. falciparum. Our findings indicated that these new triazole–quinazolinone hybrids may be considered hit molecules for further optimization studies.

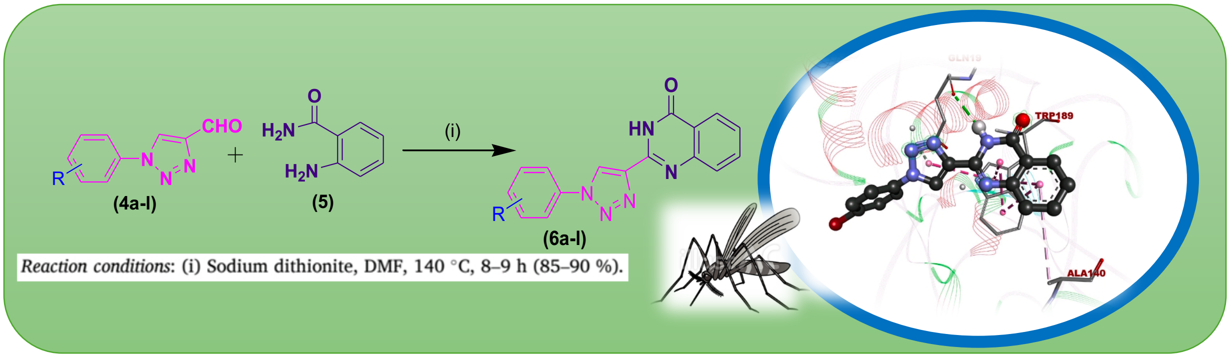

Figure1. Graphical abstract

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P-79

A Proton-Conductive Co(II)-Polyoxometalate Acts as a Precatalyst for Efficient Electrocatalytic Water Oxidation

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In this study, we demonstrate two distinct applications of a single material that are directly relevant to sustainable development: Firstly, the development of proton-conducting material for proton exchange membrane fuel cells (PEMFCs)[1] and secondly, electrochemical water splitting, where the electrocatalyst facilitates the generation of oxygen at the anode and hydrogen at the cathode in an electrochemical cell, contributing to clean energy production.[2]

A cobalt(II)-containing polyoxometalate, $[H_3O]_5[\{Co(H_2O)_4\}_3\{Na(H_2O)_4\}W_{12}O_{42}]\cdot 3H_2O$ (**Co-POM**), has been isolated in a one-step facile aqueous synthesis and characterized unambiguously using single-crystal X-ray diffraction technique along with routine spectral analyses. The paratungstate cluster anion $[W_{12}O_{42}]^{12-}$ coordinates with $\{Co^{II}(H_2O)_4\}^{2+}$ and $\{Na(H_2O)_4\}^{+}$ complex cations resulting in the formation of the water-insoluble **Co-POM** compound having three-dimensional (3-D) extended structure.

Motivated by the protonated water molecules existing as the counter cations in **Co-POM**, we conducted detailed proton conductivity studies of the **Co-POM**, achieving a value of 1.04×10^{-2} S/cm at 80 °C and 98% relative humidity (RH). The temperature- and humidity-dependent proton conductivity in **Co-POM** is governed by Grotthus mechanism with $E_a = 0.25$ eV. In addition, we have examined the electrochemical behaviour of **Co-POM**, in an alkaline borate buffer where it is found to be electrochemically unstable and acts as a pre-catalyst (and not a true catalyst) for oxygen evolution reaction (OER). A "post-mortem" analysis of the post-electrolysis sample reveals that the active species, thus formed, is a cobalt oxide material (Co_3O_4) incorporating small amounts of tungsten. Therefore, in this study, the **Co-POM** transforms into an efficient water oxidation catalyst (WOC).[3]

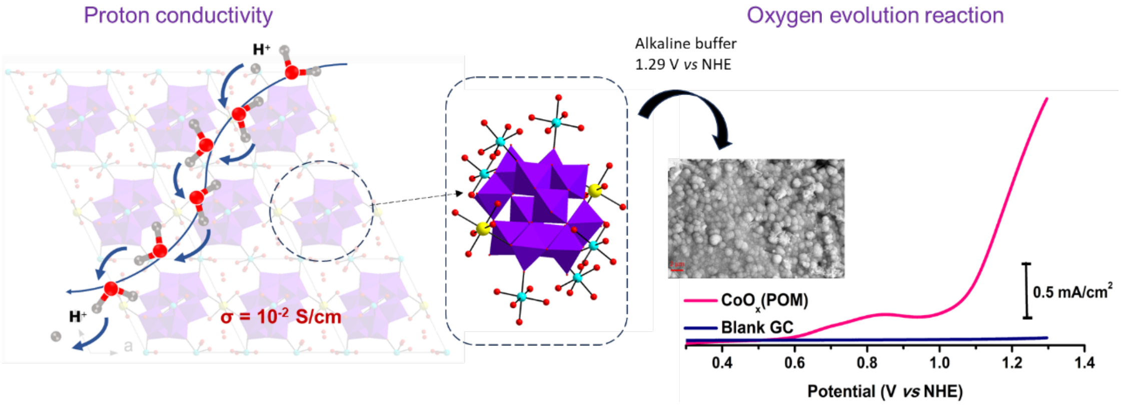

Figure 1. Schematic illustration of $[H_3O]_5[\{Co(H_2O)_4\}_3\{Na(H_2O)_4\}W_{12}O_{42}]\cdot 3H_2O$ (**Co-POM**) acting as a proton conductor and an electrocatalyst for oxygen evolution reaction (OER).

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P-80

$NdCoO_3$ nanoparticles grown on reduced graphene oxide sheets as an efficient electrocatalyst for hydrogen evolution reaction

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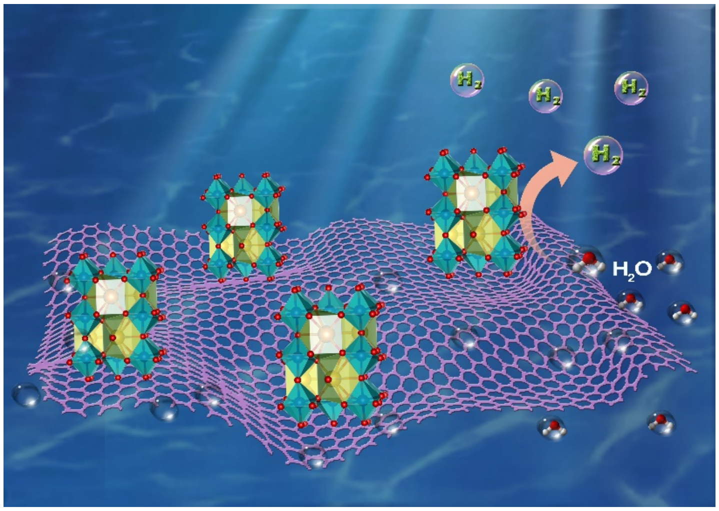
To meet the huge energy crisis due to the limitation of fossil fuel, hydrogen has been considered the most promising clean energy source due to its high efficiency, non-toxic, and clean emission products. Therefore, over the past few years, researchers have been trying to find an effective route for bulk production of hydrogen energy from water splitting. Many efforts have already been made to use suitable electrocatalysts such as transition metal-based oxides, hydroxide alloys, and carbides for hydrogen production from water splitting but these electrocatalysts are hindered due to instability over prolonged usages in alkaline solution. To overcome this issue, rare-earth perovskite oxide materials are being focussed as an efficient electrocatalyst for electrocatalytic hydrogen evolution reaction through water splitting in an alkaline medium.



In the present work, we have explored to synthesize the rare-earth perovskite neodymium cobalt oxide ($NdCoO_3$) nanoparticles grown on reduced graphene oxide (rGO) sheet, via a hydrothermal route for electrochemical hydrogen evolution in an alkaline medium. The $NdCoO_3$/rGO nanocomposite shows a remarkably low overpotential of 84 mV at the desired current density of 10 mA/cm^2, compared to pristine $NdCoO_3$ and rGO. The synergistic impact between $NdCoO_3$ and the rGO backbone, resulting in enhanced efficiency in the hydrogen evolution reaction. The nanocomposite also shows high stability and durability even more than 100 hours of electrolysis under an inert atmosphere.

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P-81

Selective Synthesis of 1,2-Dithiophene-Substituted Benzimidazoles Using Zinc Oxide Nanoparticles under Mild Reaction Conditions

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This study explores the ZnO-catalyzed cyclo-condensation between o-phenylenediamine and thiophene-2-carbaldehyde to synthesize 1,2-thiophene-substituted benzimidazoles. By altering the derivatives of both o-phenylenediamine and thiophene-2-carbaldehyde, the selectivity of the products can be controlled. It is suggested that the surface electrostatic potentials at the oxygen and nitrogen atoms of the substrates play a critical role in driving the formation of these benzimidazoles[1,2]. The optimal reaction conditions were achieved using thiophene-2-carbaldehyde (2 mmol), o-phenylenediamine (1 mmol), and 30 mg of ZnO nanoparticles in DMSO at room temperature for 8 hours. These conditions afforded excellent results, showing compatibility with functional groups such as methoxy, chloro, methyl, and fluoro. Additionally, the reaction proved effective for heteroaromatic aldehydes, delivering the desired products in moderate to excellent yields, up to 94%. The catalytic efficiency was notably enhanced by the strong affinity interactions between metal-based Lewis and Brønsted acids and the aldehyde carbonyl group, which are often employed in these catalysts.

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P-82

Selective Phosphate Removal from Wastewater with pH-Responsive Covalent Organic Networks Capable of Morphological Changes

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Phosphate is a vital nutrient for the growth of various organisms, but its increasing infiltration into aquatic environments due to human activities poses environmental risks. Recovering phosphates from wastewater is a promising strategy to combat eutrophication and conserve diminishing global phosphate reserves. To tackle this issue, we developed a pH-responsive two-dimensional covalent organic network (2D ag-CON) with multiple anion interaction sites. Upon phosphate adsorption, the surface morphology changes from spherical to sheet-like structures, a unique feature of the ag-CON. The tris-aminoguanidine-based 2D ag-CON exhibits pH-dependent adsorption and desorption properties, allowing selective phosphate capture and release by adjusting the pH of the aqueous solution. The polymer shows high selectivity for phosphate ions even with excess competing anions, with a maximum adsorption capacity (Qmax) of 719 mg/g at pH 6, and enables efficient phosphate ion release at pH ~11.5. This study highlights the development of a water-insoluble covalent organic framework that effectively captures phosphate from wastewater, helping to mitigate the adverse effects of water eutrophication.

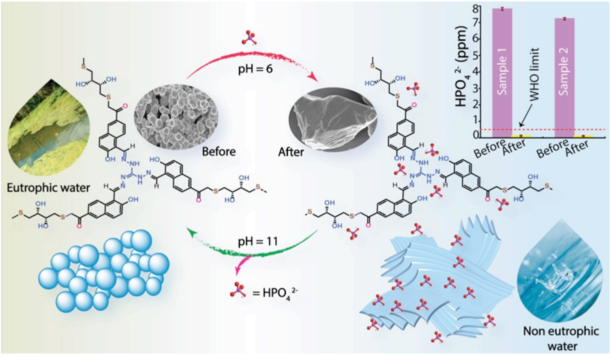

Figure. Graphical abstract of the phosphate removal mechanism from wastewater using tg-CON polymer.

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P-83

Lipase catalysed synthesis and antioxidant evaluation of dihydroindoloquinolines

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Lipase-catalyzed organic reactions have widely been carried out in the past three decades. In addition to its wide acceptance in conventional reactions such as hydrolysis (1), transesterification (2) and enantiopure synthesis (3) (kinetic resolution and dynamic kinetic resolution) several reports on the catalytic promiscuity of lipases have also been published. The concept of promiscuity, where lipase catalyzes reactions beyond its natural function, has been perceived as a useful phenomenon which can enhance the utility of lipase as a biocatalyst. Indoloquinolines and dihydroindolquinnolines have known to have various biological activities such as antimicotic, antihyperglycemic and cytotoxic properties and antitumor activity etc.

This work investigates the synthesis of dihydroindoloquinolines utilizing immobilized lipases as biocatalysts. Among the various lipases screened, Candida rugosa lipase exhibited the most promising results, achieving moderate to good yields across a range of substrates. Optimization of reaction conditions revealed that the optimal temperature for most substrates was 35 °C, with a few substrates performing best at 40 °C. Additionally, an ethanol/water mixture was identified as the most effective solvent combination for the transformation. Several synthesized dihydroindoloquinolines analogues were evaluated for their biological activities, demonstrating significant antioxidant properties alongside mild antibacterial and antidiabetic effects.

These findings highlight the utility of lipase-catalyzed reactions in the synthesis of bioactive compound.

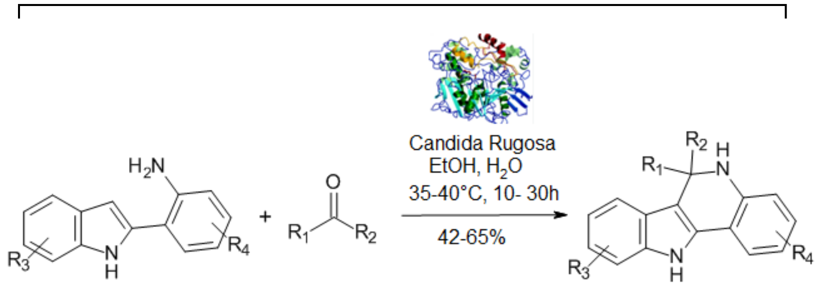

Figure 1. General scheme for synthesis of dihydroindoloquinolines using lipase.

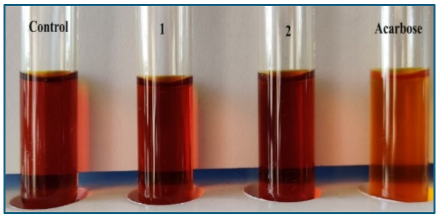

Figure 2. Antioxidant activity of synthesized compoundsby % DPPH free radical scavenging.

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P-84

Tarnish Resistance Mechanism in Ag-4Cu-2.5Zn-1Ge novel Alloy: A Comprehensive Experimental and Computational

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Silver and its alloys undergo tarnishing with time, which is a black stain on its surface which diminishes the luster. The reaction of atmospheric Sulphur with Silver causes the formation of Ag_2S compound that gives the black colour. Developing a tarnish resistant silver alloy was attempted by many researchers by alloying silver with oxidizing elements that form a passive oxide layer on the surface and prevent the Ag_2S formation. The element germanium is proven to provide better tarnish resistance to sterling silver alloy (92.5wt.% pure) which is commercially exploited and available under the trade name of Argentium© However the mechanism behind its tarnish resistance behaviour is still unknown. In the present work, the tarnish resistance behavior of silver alloy containing copper, zinc, germanium, and boron was investigated. The alloys were prepared by melting and casting route, followed by passivation heat treatment (PHT) to create the oxide layer. Accelerated tarnish test was carried out to the alloy as a function of time to investigate its tarnishing behavior The temperature for PHT was optimized using Thermogravimetry Analysis (TGA) for various isothermal durations. And to more accurate the time and temperature of PHT were optimized by investigating the passive oxide layer formed systematically using micro-Raman spectroscopy. In our present study high tarnish resistance was obtained for the Ag-4Cu-2.5Zn-1Ge which was confirmed by the light reflectivity measurement used for the samples exposed to accelerated tarnished testing environment. The mechanism behind the tarnish resistance of the present composition was derived using Density Functional Theory (DFT) by comparing sulphide and oxide binding energies (BE) on these alloys. The composition Ag -4.2Cu-2.8Zn 1.4Ge has S2 (B.E)/ O2 (B.E) of about 132% which is much less than the ratio of 222% for pure silver.

P-85

Palladium-Catalyzed Substrate-Switchable *ortho*-C-H Alkenylation and Alkylation of Benzoic Acids using MBH Alcohols

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A Pd-catalyzed, weak carboxylate-directed *ortho*-C-H alkenylation and alkylation of benzoic acids has been developed, utilizing MBH alcohols as coupling partners. This approach distinguishes itself from previous methods, which predominantly yielded allyl products. The alkenylation pathway leads to the formation of α,β-unsaturated aldehydes, while the alkylation strategy produces β-ketoesters. This method showcases substrate-switchable reactivity, broad functional group tolerance, a diverse substrate scope, and facilitates late-stage diversification.

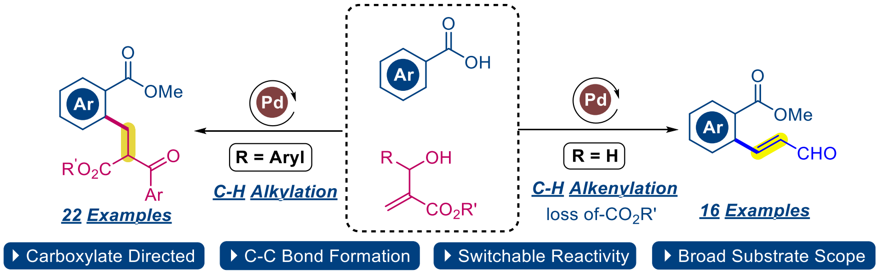

Figure 1. MBH Alcohol-Switchable *ortho*-C-H Alkenylation and Alkylation of Benzoic Acids.

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P-86

In silico Investigation of β-Lactams as Possible Inhibitors of Spike Protein RBD of SARS-CoV-2

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The deadly impact of COVID-19 was undoubtedly the worst threat of the 21st century so far, which resulted more than 6.9 million deaths and 767 million confirmed cases [1]. The pandemic was caused by a novel virus named SARS-CoV-2, specifically belonging to the β group of the Coronaviridae family [2]. The unavailability of specific drug to neutralize SARS-CoV-2 is still a matter of concern to the society. The evolution of new variants of SARS-CoV-2 adds more trouble [3-6]. In this context, repurposing and thereby discovering drugs and designing new potential drug molecules with rapid clinical translatability is really necessary but significantly challenging. Among various essential proteins of SARS-CoV-2, spike protein has been a prime choice for drug and vaccine development due to its role in binding with hACE2 for viral infection [7]. This presentation represents the investigation of our earlier reported β-lactam compounds as lead molecules to inhibit the spike RBD-ACE2 interaction.

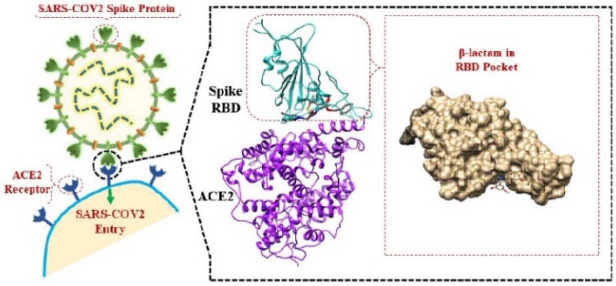

Figure 1. Graphical abstract of the β-lactam inhibiting spike RBD-ACE2 interaction

We have selected sRBD as our drug target and performed detailed *in-silico* studies to check the activity of multiple β-lactam compounds derived from penicillin. To check the greater efficacy of our compounds against diverse variants of SARS-CoV-2, we selected sRBD of Wuhan, Delta and Omicron variants of SARS-CoV-2. First, we checked the ADME properties of the molecules. Then, we carried out molecular docking of the compounds with the three different variants of sRBD. To further validate the stable interactions, MD simulations for 100ns of the best-docked complexes were performed. Following our computational investigation, we have designed and proposed a series of novel β-lactam compounds as potential sRBD inhibitors of Wuhan, Delta and Omicron variants of SARS-CoV-2.

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P-87

Manganese-Complex Catalyzed Sequential Multi-component Reaction: Enroute to a Quinoline-Derived Azafluorenes

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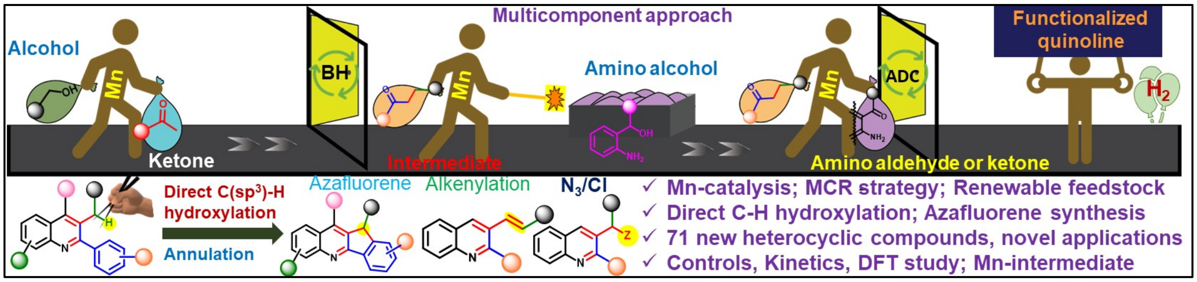
Developing highly functionalized heterocyclic scaffolds via dehydrogenative multicomponent reactions (MCRs) is an emerging area in catalysis. However, it is underexplored because it necessitates the development of new efficient catalysts having high selectivity to direct the reaction in order to achieve a high amount of desired polyfunctionalzied heterocycles while minimising the possibility of multiple side reactions. Herein, we introduced a new MCR approach to synthesize poly functionalized quinolines. This current protocol covers a broad range of substrate scope, including various challenging primary and secondary alcohols, providing genres of highly functionalized complex quinoline motifs.



Furthermore, an unprecedented direct C(sp^3)-H bond hydroxylation of the product provides a new scope to construct medicinally relevant azafluorene derivatives. We investigated a series of control, kinetics, and DFT studies to comprehend the detailed reaction route and the catalyst's function in the MCR sequence. Computational studies reveal that dehydrogenation of amino alcohol could be the rate determining step in our MCR strategy and water assisted Mn-H complex formed a more stable transition state which travels via 7.4 kcal/mol lower energy barrier than amino alcohol assisted transition state to generate the active amido complex.[1]

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P-88

Precise Identification of the LUMO in Silanes: A Key to Understanding Molecular Properties

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The Silicon analogs of hydrocarbons are called silanes. Due to extensive sigma delocalization, linear silanes show various semiconducting and photo-conducting properties. To use these properties, we need to have a clear understanding of their electronic structure. The frontier orbitals of saturated silanes have generated significant amount of interest in theoretical chemistry. The unfilled orbitals of linear silanes are unbound in nature. The LUMO obtained from the SCF solution is very tricky as it exists among large number continuum states with identical energies. Parametric equations of motion [1,2] in conjunction with nuclear charge stabilization method has been implemented for precise identification of the LUMO.

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P-89

Remote control of supramolecular organization of butylated PNI

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Control on the properties of a system from a remote location via signal transduction is a good method to encourage an artificial system to follow biological mechanisms, where many essential biological functions are achieved through indirect signalling input between two different systems. To achieve such an objective, the molecule **butylPNI**`was synthesized, which undergoes aggregation in non-polar solvents to provide flexible fibres. The self-assembled structures of this dye also show interaction with fullerenes,and acids (TFA and TfOH). The interaction is different for either of the acid. In a system consisting of all three components of **butylPNI**, C60 and TFA, the effect of TFA on **Agg**$^{\mathbf{BuPNI}}$ dominates and the absorption spectra indicates a supramolecular arrangement corresponding to TFA$\subset$**Agg**$^{\mathbf{BuPNI}}$.

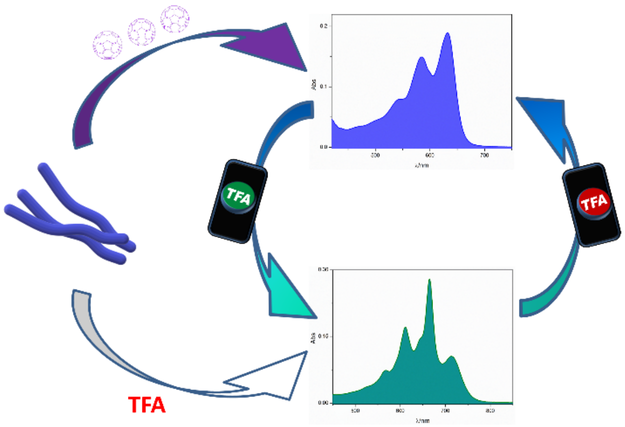

Figure 1. Diagrammetic representation for remote switching of supramolecular organization.

Reversible switching of the supramolecular arrangements between C60-**Agg**$^{\mathbf{BuPNI}}$ and TFA$\subset$**Agg**$^{\mathbf{BuPNI}}$ is achieved via change in the pH of an adjacent aqueous layer, situated below the organic layer (95:5 MCH:toluene) composed of the C60-**Agg**$^{\mathbf{BuPNI}}$. Movement of the acid occurs by the mechanism of diffusion through the bilayer. This method eliminates production of any unwanted salt or chemical waste in the organic layer and thus is both spectroscopically and chemically reversible.

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P-90

Substituent-dependent, Switchable Synthesis of Non-aromatic and Aromatic Heterocyclic Sulfones Using Visible Light

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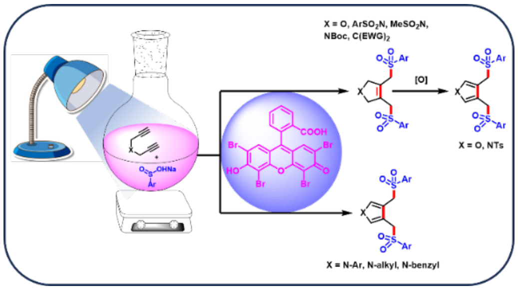
In this article, we described a visible-light-induced switchable synthesis of non-aromatic and aromatic sulfonyl heterocycles. The product selectivity between 2,5-dihydropyrrole and pyrrole can be tuned by altering the substituent on the N-atom of 1,6-diyne. We highlight the intricacy and efficiency of this approach in constructing molecular frameworks under mild conditions with high functional group tolerance. This study elucidates the mechanism underlying product selectivity, highlighting its potential as a compelling alternative to traditional synthetic techniques.



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P-91

Sulfur Ligated Iron(III)-Alkylperoxide Complex: Spectroscopic Insights and Mechanistic Studies of Electrophilic Hydrogen Atom Abstraction with Aldehydes

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Nonheme iron dioxygenases often utilize a co-substrate, such as α-ketoglutarate, to generate a high-valent iron(IV)-oxo species in their catalytic cycle. It has been proposed that this biosynthesis reaction happens via the transformation of an iron(II)-α-ketoglutarate complex with dioxygen into iron(III)-persuccinate that rapidly forms an iron(IV)-oxo(succinate) species by the expulsion of CO_2. However, these enzymatic iron(III)-alkylperoxo complexes have never been trapped and characterized for the α-ketoglutarate-dependent dioxygenases and therefore their contribution to biocatalysis remains controversial. In biomimetic chemistry it has been challenging to use dioxygen as the oxidant and, therefore, researchers commonly use iron(III)-alkylperoxo complexes instead. To resolve the controversy of iron(III)-alkylperoxo reactivity, we report here the synthesis, characterization and reactivity of a novel thioether ligated iron(III)-alkylperoxo complex with a pentadentate N4S ligand system. The iron(III)-alkylperoxo complex was characterized with UV−vis absorption spectroscopy, resonance Raman spectroscopy, Electron Paramagnetic Resonance spectrometry, and electrospray ionization mass spectrometry. The complex shows electrophilic reactivity with triphenylphosphine and cyclohexanecarboxaldehyde (CCA) as model substrates. The comprehensive mechanistic insight into its reaction with CCA indicates a novel aldehydic-H atom abstraction to give cyclohexanecarboxylic acid as product. The detailed mechanistic studies and computational work reveal a homolytic O−O bond cleavage from the iron(III)-alkylperoxo to form a putative iron(IV)-oxo complex during the catalytic process. To the best of our knowledge, the present study reports the first example of a mononuclear low-spin ($S = ½$) non-heme iron(III)–alkylperoxo complex showing unprecedented electrophilic reactivity in oxidation reactions.

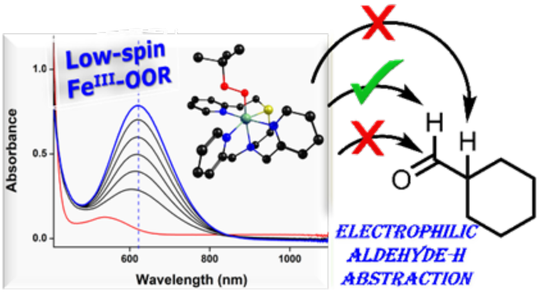

Figure 1. Graphical abstract of for the reaction of cyclohexanecarboxaldehyde with Fe^{III}-OOR species.

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P-92

Metal-Metal Oxide Nanoparticle Embedded Ecofriendly Film with Natural Enhancers for Food Preservation

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The devastating usage of non-degradable plastics in our day-to-day lives has made a huge negative impact on our ecosphere. Numerous cases related to the reparations to the flora and fauna due to plastic wastes are being recorded [1]. Single-use plastics used for storing food products also contribute to the overall pollution. To minimise their effect, a biodegradable replacement is needed. Packaging films made with a polymer like polyvinyl alcohol (PVA), combined with metal oxide nanoparticles, result in an environmentally friendly packaging material with enhanced functional properties [2]. The current work involves utilising low content of PVA embedded with Mg-ZnO nanoparticles (≈ 32 nm) and incorporating agro waste (rice bran and *moringa* fibre) for the film matrix, to improve their beneficial value while maintaining their physical parameters, making the film unique and suitable for increasing the shelf life of the food [3,4].

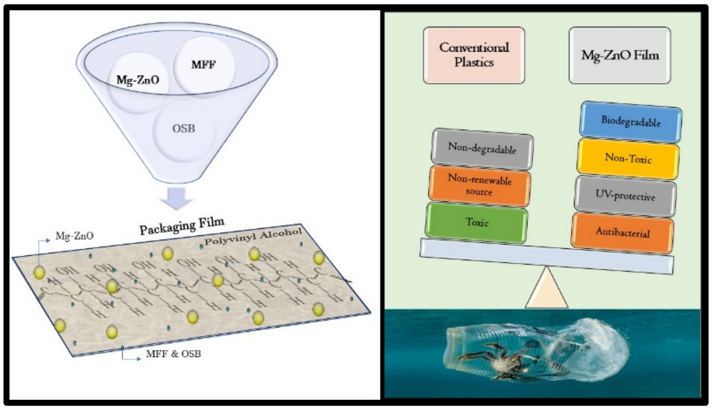

Figure 1. Graphical abstract of the prepared film and its merits

The Films were prepared using the solvent-cast method with varying ratios of nanoparticles (2, 4, 6 & 8 w/w%) and their structural properties were analysed using XRD, optical properties using UV-spectroscopy and their antibacterial efficacy were compared. The incorporation of Mg-ZnO nanoparticles enhanced the film's overall efficiency, making it a better replacement for conventional plastic food packaging material.

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P-93

Modulating Hydrogen Bubble Adhesion for Improved Water Splitting

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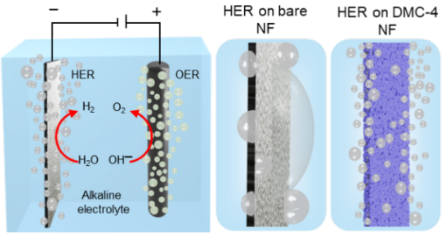
In the realm of electrochemical hydrogen evolution reactions (HER), the produced gas bubbles often suffers from adhesion to the electrode surface. This bubble adhesion can significantly hinder the overall reaction performance by obstructing the active catalytic sites that are essential for the efficient conversion of water into hydrogen.[1] Over the years, a wide range of catalysts have been developed and optimized to enhance the efficiency of HER by improving the activity, stability, and durability of the catalytic materials.[2] However, despite these advancements in catalyst design, the issue of gas bubble adhesion remains a critical obstacle. The presence of bubbles not only reduces the effective surface area of the electrode but also introduces mass transport limitations, thereby lowering the overall efficiency of the system.. To dislodge nucleated bubbles, buoyancy forces need to surpass the capillary forces, indicated by ratio of these forces, Eötvös number (Eo) exceeding 1. Herein, we report a universal chemically reactive multilayer coating on an electrode to chemically modulate the adhesion force of nucleated gas-bubble on the electrode. A dual-modified coating on a Ni-foam substrate, provided non-adhesive superaerophobicity, resulting in a remarkably low nucleated bubble adhesion force of 4.6 ± 0.3 µN. This dual modified Ni-foam electrode significantly improved hydrogen evolution, lowering overpotential (333 to 249 mV at 100 mA cm^{-2}) and boosting current density (680 to 1270 mA cm^{-2}) compared to a bare Ni-foam. The chemical modification of Ni-foam expedites the removal of tiny hydrogen bubbles (minimum size 0.64 mm, Eo = 0.05), preserving catalytic sites for superior HER, with a remarkable 98.2% faradaic efficiency. This approach also proved effective on other electrode types.



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P-94

A well-designed bimetal coordination networks for efficacious electrochemical detection of caffeine in beverages

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Caffeine (CAF) is a naturally occurring alkaloid, it is chemically known as 3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione or 1,3,7-trimethyl xanthine, derived from the N-methyl derivative of xanthine. As a heterocyclic compound containing nitrogen, it exhibits the basic properties of an amine. Found in various plant materials like tea leaves, cola nuts, coffee beans, cacao beans, and pharmaceutical drugs, and it acts as a central nervous system (CNS) stimulant [1]. However, excessive amount of CAF consumption leads to negative effects such as anxiety, heartburn, seizures, bone mass loss, elevated blood pressure, cardiovascular issues, hyperactivity, and kidney diseases [2, 3]. Therefore, monitoring CAF levels is crucial for confirming the quality and safety of food products and become a significant focus for researchers.

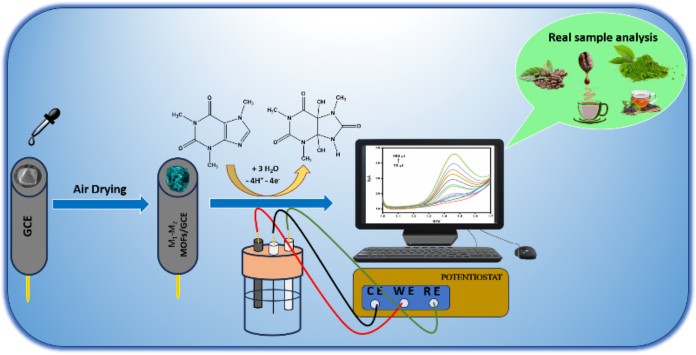

Figure 1. Graphical abstract of electrochemical detection of CAF.

Herin, we developed a novel bimetal organic framework (M1-M2 MOFs) was synthesized by a one-pot hydrothermal method. And modified with glassy carbon electrode (GCE) were used for the electrochemical detection of caffeine (CAF) and thoroughly characterized towards its physicochemical and electrochemical properties. The results show an octahedral-shaped M_1-M_2 MOFs with a surface area of 100.471 m^2/ and the electrochemical studies were carried out using Britton-Robinson buffer solution (B-R buffer) of pH 3.0. The results show good electrocatalytic activity within the linear range of 0.1 to 1.5 µM, exhibited a low detection limit (LOD) of 0.098 µM and a limit of quantification (LOQ) of 0.327 µM. This is due to the large electroactive surface area, significant mass, efficient ionic transport, synergistic effects, and chemical stability of prepared M_1-M_2 MOFs contributing to its efficient sensing of CAF. In addition, M_1-M_2 MOFs /GCE show excellent reproducibility, stability, and selectivity. Overall, it becomes a promising electrocatalyst for the quantification of CAF for real-time practical analysis.

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P-95

Packing polymorphism and symmetry non-equivalence in Co(II) complexes of flexible dicarboxylic acid of 4,4'-biphenol

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Crystal polymorphism is an extremely attractive topic, the main reason being that although composed of the same units/entities, different polymorphic forms can have different physical, chemical and mechanical properties.[1,2] In this research work, structures of three new polymorphic (P1, P2 & P3) forms of [Co(II)(4-bpa)$_2$(py)$_3$H$_2$O](4bpa= 2,2'-([1,1'-biphenyl]-4,4' diylbis(oxy)) diacetic acid as the ligand, py=pyridine as the ancillary ligand and Co(II) as the metal center, have been synthesized and characterized by FTIR, NMR and single X-Ray crystallographic technique. The differences in architectures of the polymorphs are attributed to differences in its packing arrangements in the lattice. The different crystallographic structures arise at the intermolecular level, being determined by different intermolecular interactions as seen in the three polymorphic forms, which differ in shapes, sizes and saturation. Another unique property is showing symmetry non-equivalence [3] in the lattice of two of the polymorphs (P1 &P2) and P1 & P2 crystallize in a triclinic system with P-1 space group, while P3 shows monoclinic crystal system with C2/c space group. TGA, DSC studies and its temperature dependent magnetic susceptibility of the polymorphs have been conducted.

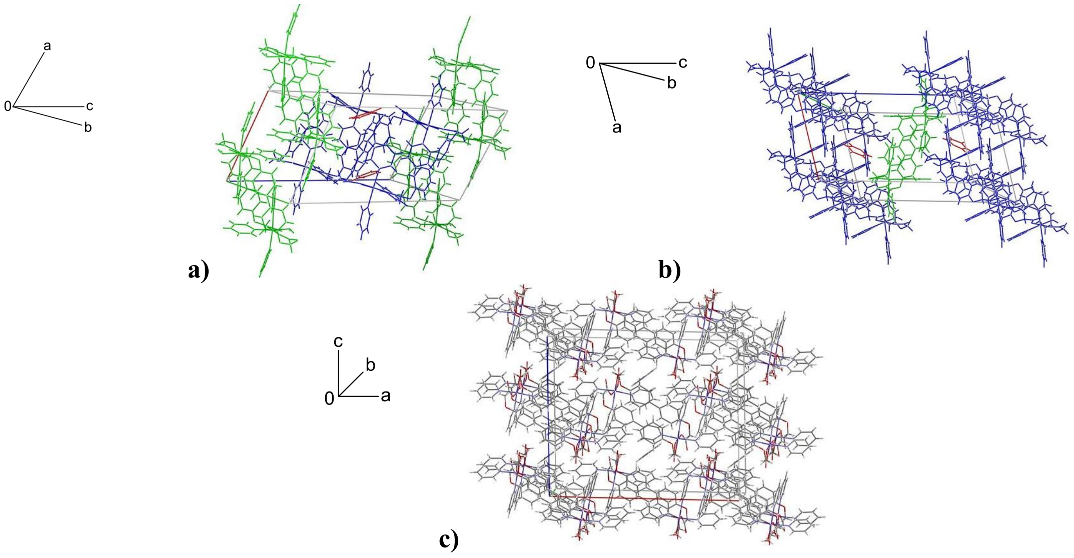

Figure 1: a), b) and c) show different crystal packing arrangements in P1 & P2 (with symmetry non-equivalence) and P3 polymorphs respectively.

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P-96

Synthesis of imines from the coupling reaction of alcohols and amines catalyzed by phosphine-free cobalt(II) complexes

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Phosphine-free, air stable cobalt(II) based complexes (1a and 1b) consisting of ligands **L^1H2** and **L^2H2** (**L^1H2** = N,N'-((1,2-phenylenebis(azaneylylidene))bis(methaneylylidene))diphenol and **L^2H2** = N,N'-bis(4-diethylaminosalicylidene)-4,5-dichloro-1,2-phenylenediamine) were synthesized and utilized as catalysts in the coupling reaction of alcohols with amines into imines following an acceptorless dehydrogenative pathway. The reactions were carried out in the presence of *t*-BuOK base with low catalyst loading (1 mol%) in an open atmosphere. The corresponding imines were isolated in moderate to excellent yields. The methodology was screened with different substituted alcohols and amines. The proposed mechanistic pathway of this reaction was ascertained through intermediate mass and ^{1}H NMR analyses.[1] Most of the previously reported 3*d* transition metal catalysts used in imine synthesis reactions have a phosphine ligand environment, and the reactions were performed under inert conditions.[2-4] Herein we have developed a sustainable route for the synthesis of imines from the coupling reaction of alcohols with amines under aerial reaction conditions using phosphine-free air stable cobalt catalysts.

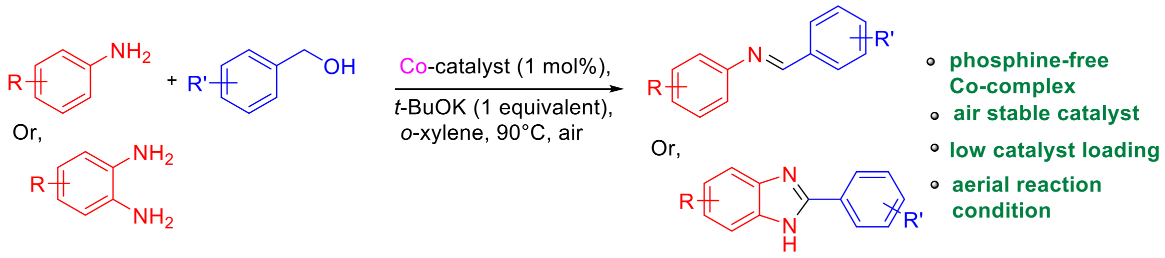

Figure 1. Graphical abstract of imine and benzimidazole derivatives synthesis using cobalt-catalyst

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P-97

Living photo-oligomerization behavior of diazaanthracene-derived macrocycle

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Macrocycles occupy a very prominent space in supramolecular chemistry due to their well-defined cavity suitable for molecular recognition, sensing, catalysis, etc.[1,2] Recently, stimuli-responsive macrocycles have gained significant attention because of their reversible dynamic function.[3] Among the various stimuli, light serves as an ideal candidate because of its tunability over a wide range of wavelengths, noninvasive nature, and, most importantly, the fact that it avoids the generation of waste compared to other responsive systems.[4] In this regard, the integration of photo-responsive components into macrocycles and subsequent light-induced oligomerization of those has been an attractive and efficient approach for the preparation of carbon-rich covalently linked macromolecules.[5] However, capturing intermediate oligomers in photopolymerization reactions to study their properties often proves challenging. We intended to use the classic [4+4] cycloaddition reaction of anthracene and extend it to the 1,8-diazaanthracene system which also shows similar behavior. However, interestingly, it gives an *anti-parallel* photodimer, minimizing the dipolar repulsion from the endocyclic nitrogens.[6] Taking advantage of this phenomenon, we prepared a planar aromatic oligoamide macrocycle comprising 1,8-diaza-anthracene unit which undergo efficient photo-oligomerization in a stepwise manner through intermolecular *anti-parallel* photodimerization of 1,8-diaza-anthracene. We strategically tuned the side chains to control their regioselectivity, favoring the *exo*-product over the *endo*-isomers. We were able to isolate and completely characterize the oligomers up to octamer having molecular weight >10 kDa, which is close to the molar mass of some low molecular weight polymers.[7] Additionally, the oligomers retained sufficient photoreactivity to undergo further oligomerization, either by themselves or by adding fresh monomers, exhibiting living polymerization-like behavior which leads to the statistical enhancement of the population of the higher oligomers, which is otherwise not easily accessible. These oligomers are thermally reversible, allowing the recovery of monomers. Our findings demonstrate an efficient approach to generating higher molecular weight oligomers in a single-step process, which can be valuable for optoelectronic materials.

Keywords

Macrocycle, 1,8-diazaanthracene, photo-oligomerization, living oligomers.

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Controlling Energy of LUMO from Remote Site and it's Effect on Electrochemical Property and Oxygen Atom Transfer Reactivity and O-H bond activation by Cu(II)-Nitrite Complexes

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Nitric oxide (NO) generation from Nitrite (NO_2^-) reduction is of significant interest as NO is an important signalling molecule which play vital role in controlling blood flow and oxygenation. In biology, NO_2^- to NO conversion is performed by Cu-nitrite reductase reduces while alternatively NO_2^- reductio to NO can be performed at copper center via oxygen atom transfer (OAT) to electron rich substrate like PPh_3. During this OAT reaction by synthetic Cu^{II}-NO_2^- complex, PPh_3 is oxidized by two electrons to O=PPh_3 while Cu^{II} gets reduced to Cu^{I} with simultaneous reduction of NO_2^- to NO. Thus, LUMO of Cu^{II}-NO_2^- is expected to play a significant role in the OAT reactivity of Cu^{II}-NO_2^-. This work describes systematic tuning of LUMO energy by remote site modification of ligand which leads to systematic change in electrochemical property and OAT activity of Cu^{II}-NO_2^-.

For this purpose, we describe here four Cu^{II}-NO_2^- complexes: $[Cu^{II}(L_{CH2})(NO_2)(ClO_4)]$ (**1**), $[Cu^{II}(L_O)(NO_2(ClO_4)]$ (**2**), $[Cu^{II}(L_{CH2}^{Me})(NO_2)(ClO_4)]$ (**3**), $[Cu^{II}(L_O^{Me})(NO_2)(ClO_4)]$ (**4**) which have closely similar primary coordination sphere but they have different substituents at remote site. We apply this approach of controlling LUMO energy for OAT reaction as well as O-H activation reaction with copper(II) nitrite complexes. For both the OAT and O-H bond activation reaction, on going from complex **1** to **4** there is increase in reactivity of metal complexes only by changing the second coordination sphere. The reaction mechanism for both the OAT and O-H activation processes is explored with combined kinetic analysis and computational study.

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P-99

Cooperative Rh/Chiral Phosphoric Acid Catalysed Diastereo- and Enantioselective [3 + 3] Cycloannulation: Access to Oxa-Bridged Indoles

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Cyclohepta[*b*]indole structural motifs are present in many natural and non-natural compounds with important biologically activities.[1] For instance, arcyriacyanin A, a cytotoxic compound that inhibits protein kinase C and protein tyrosine kinase, was isolated from Arcyria nutans.[2] Murraya exotica roots were used to extract exotins A and B, which showed inhibitory effects on lipopolysaccharide (LPS)-induced nitric oxide (NO) production in BV-2 microglial cells.[3] The alga Caulerpa serrulata, which is native to the maritime environments surrounding the Paracel Islands, yielded the bisindole caulersine.[4] It inhibits the multixenobiotic resistance pump in algae and acts as plant growth regulator. New class of histone deacetylase (HDAC) inhibitor, is one of the most potent compounds described (IC_{50} =63 nM), 500 times more effective than previously recorded inhibitors.

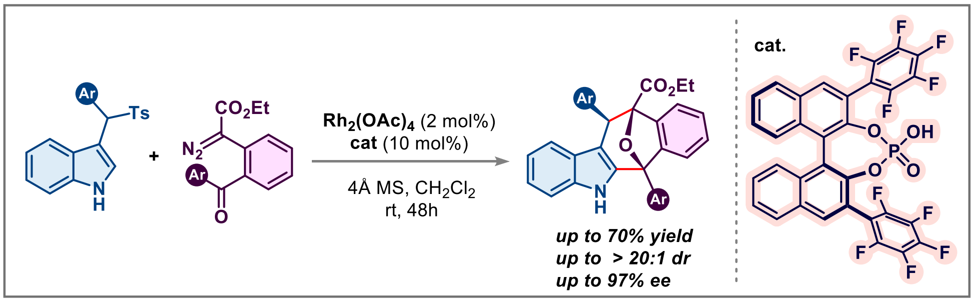

Figure 1. (3+3) cycloannulation reaction

A catalytic asymmetric (3+3)-cycloannulation reaction between in situ formed carbonyl ylides[5,6] and indole-embedded α, β-unsaturated imines for the preparation of oxa-bridged cyclohepta[b]indoles with excellent yields and stereoselectivity in a single synthetic step. The combination of rhodium and chiral phosphoric acid catalysis working in concert to generate both transient intermediates in situ provides direct access to complex bicyclic products with two quaternary and one tertiary stereogenic centers. [6]

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P-100

Impact of Gadolinium Phosphate ($GdPO_4$) and Various Cations (Li^+, Ca^{2+}, La^{3+}) on the NIR Reflectance of Bismuth Vanadate Pigment

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Bismuth vanadate ($BiVO_4$) pigments are known for their bright yellow colours and durability. Furthermore, doping and composite formation with other rare earth elements can help to improve their (NIR) reflection properties. Adding gadolinium phosphate ($GdPO_4$) to bismuth vanadate ($BiVO_4$) pigments makes better their NIR reflectance, a crucial feature for particular applications that require less heat build-up. Similarly doping of $BiVO_4$ with Li, Ca, and Mo improve its NIR reflection properties. These dopants slightly changes $BiVO_4$'s electronic structure and crystal parameters, leads to its ability to reflect heat radiation. The addition of rare earth metal oxides in these pigments extremely effective at maintaining the surfaces cool when it exposed to direct sunlight.

This study explores the effects of $GdPO_4$ and a combination of Li, La, Ca, and Mo ions on the reflectance properties of Bismuth vanadate (BiVO4), a well-known yellow pigment, using scheelite-type solid solutions. The powdered pigments have a monoclinic scheelite (s-m) type structure. [(Li0.33Ca0.33La0.33)*x*Bi1-*x*][Mo*x*V1-*x*]O4 [1] and (BiV)1-*x*(GdP)*x*O4 [2]. When $GdPO_4$ and the multi-ion system are incorporated into the $BiVO_4$ structure, a structural transition is brought about that impact the optical properties, such as bandgap tuning and absorption edge shifts. With particular colour coordinates displaying the most vivid hue at b* = 65.42 in the $GdPO_4$ system and b* = 78.32 in the multi-ion system, these pigments produce a range of intense yellow shades. They also have a high near-infrared reflectance, which makes them perfect for use as environmentally friendly and sustainable cool colourants in surface coating, paint, and plastic applications. These findings highlight the potential of [(Li0.33Ca0.33La0.33)*x*Bi1-*x*][Mo*x*V1-*x*]O4 and (BiV)1-*x*(GdP)*x*O4 as eco-friendly colorants for various applications which includes, surface coatings, paints.

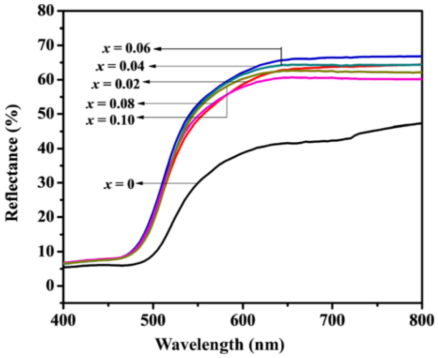

Figure 1. Reflectance spectra of (BiV)1-*x*(GdP)*x*O4 (*x* = 0, 0.02, 0.04, 0.06, 0.08 and 0.1).

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Low-valent Post Transition Zinc Metal Catalyst Bearing C-C Bond Formation Reactions

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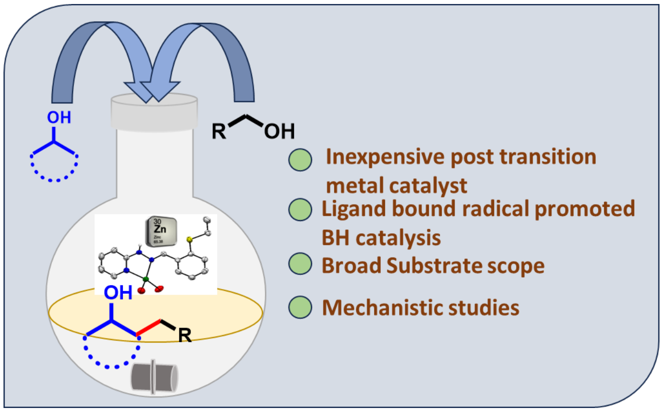
Well-defined and bench stable hydrazenyl ligand based bidentate zinc catalysts were prepared and catalytic activity was checked towards C-C bond formation reaction. Mechanistic study revealed that catalyst undergoes 1e$^-$ reduction process by KO^{t}Bu to produce ligand bound radical as an active catalyst for C-alkylation reaction. A wide range of substrate scope has been demonstrated with array of secondary alcohols and primary alcohols. With application of gram scale production, challenging steroid molecule and diverse functional group bearing alcohols were chemo-selectively alkylated via this method. Detailed control study supported hydrogen atom transfer (HAT) relay the dehydrogenation of alcohols and control experiments incorporating deuterium labelling to the alcohol acclaimed the borrowing hydrogen (BH) pathway for the catalytic cycle. Radical quenching experiment endorse the radical pathway in catalytic cycle. Kinetic study underpins the first order reaction profile was followed with respect to alcohol.



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P-102

Microscopic, Spectroscopic and Thermophysical Properties of *Cocus nucifera* Mediated Graphene Nanomaterials

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In recent years, graphene and graphene-based nanomaterials have emerged as a promising new class of sophisticated carbon functional materials with exceptional electrical, optical, mechanical, and chemical capabilities. The present work focused on single pot aqueous synthesis of graphene through a green route by reduction of graphite powder using biogenic reducing agent, *cocus nucifera* coconut water as a rich source of antioxidants along with $NaNO_3$,H_2SO_4,$KMnO_4$,$H_2O_2$and deionized water respectively at low temperature (35°c).The end product (1.2797g) exhibited Ultraviolet –visible spectral peak at $\lambda_{max} = 264$ nm,[1] indicating the presence of π- conjugation leading the observed peak towards the longer wavelength region. Fourier Transform Infrared spectroscopy revealed prominent peaks at 2948.2 cm^{-1} and 2855 cm^{-1} representing C-H stretching of methylene groups.[2] From Dynamic light scattering spectroscopy intensity size distribution or Z-average diameter of 446.2 nm was obtained from the auto correlation function using the general purpose mode for the materials. Poly dispersivity index, 0.612 indicating wider particle size distribution in the dispersion medium. From thermal gravimetric analysis carbon decomposition with reference to its temperature of maximum mass change rate (Tmax. = 698˚C) has been observed indicating the formation of pure graphene.[3] X-ray diffraction spectrum exhibited a strong peak at ca. 26.5˚C (2θ) corresponding to 002 crystal lattice indicating graphite reflections.[4] d-spacing and crystallite size was calculated as 0.34 nm and 28.22 nm .Uniformly exfoliated graphene and their wrinkled pallets / nanosheets that are transparent to the electron beam at low magnification were observed in HRTEM and FESEM micrographs.[5].Raman spectroscopic study indicated D and G bands in between 1200 – 1600 cm^{-1}. I_D / I_G ratio was calculated to be 1.16, indicating the formation of multilayered graphene occasionally. The 12D/I_G was calculated to be 1.84, indicting the formation of double layered graphene. By using Tuinstra Koenig Relation, the crystalline size was found to be 11.73 nm (λ_L=488 nm, I_D/I_G ratio = 1.16.[1] The XPS spectrum of graphene showed a highly intense band at 284.7 eV, C 1s spectra. Peaks at 285.1 eV, (C-O), 287.1 (C=O) and 288.3 eV (O-C=O) were also observed.[6]. In order to study the thermo-physical properties of prepared graphene, its nanofluids were prepared by two step method in various ionic and non ionic base fluids. Sodium dodecyl sulfate and cetrimonium bromide were used as surfactants to manipulate the size and functionalize the nanomaterials under investigation for complete dissolution in the respective based fluids. Various parameters like molar volume, viscosity and thermal conductivity are under investigation. In the present work density of nanofluids of graphene at temperature (20-80ºc) in various base fluids are discussed.

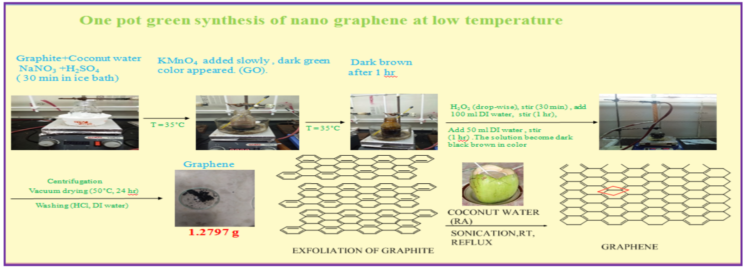

Figure 1. Graphical representation of Cocus nucifera mediated graphene nanomaterial.

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P-103

A Versatile Pd-Catalyzed Alkyne Annulation Process for π-Extended Benzofulvene Synthesis

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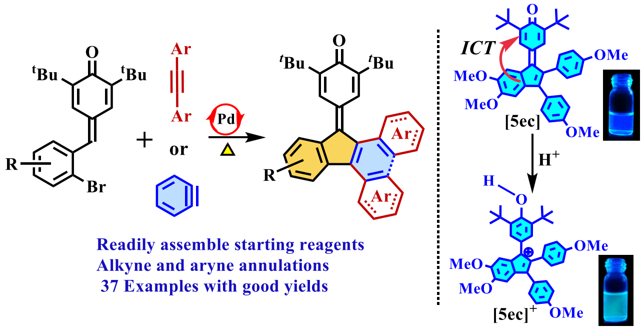
p-Quinone methides (*p*-QMs) is well recognised amongst the synthetic community due to its electrophilic propensity and unique 1,6-reactivity patterns with various range of nucleophiles for synthesis of heterocyclic systems, natural products and various bioactive molecules.[1] The derivatives, *ortho*-aminophenyl and *ortho*-hydroxyphenyl-substituted *p*-QMs are well employed for various alkyne-based annulation and cascade 1,6-addition/[4+2] cyclization processes to construct chromene and xanthene frameworks.[2]



Readily assemble starting reagents
Alkyne and aryne annulations
37 Examples with good yields

Scheme:1 Synthesis of π- extended benzofulvenes *via* cascade annulation of alkynes with *p*-QMs.

Additionally, there are also [3+2] cascade alkyne annulation and [2+2] annulation/retro-4π electrocyclization/ imino-Nazarov cyclization combined reactions to access spirocyclic cores and aminoindene derivatives respectively.[3] However, exploration of alkyne annulation with *ortho*-bromophenyl *p*-QMs through tandem process is yet to be explored. The implementation of this method helps to access the π-extended benzofulvene derivatives which have remarkable usefulness in biological as well as in material sciences.[4] Thus, we have reported a simple and straight forward Pd-catalyzed cascade alkyne/aryne annulation of *ortho*-bromophenyl-substituted *p*-quinone methides which via C-C bond formation followed by 1,6-addition reaction affords diverse functionalized π-extended benzofulvenes.

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P-104

Novel molecular hybrids of EGCG and quinoxaline: Potent multi-targeting antidiabetic agents that inhibit α-glucosidase, α-amylase, and oxidative stress

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Diabetes mellitus is a multifactorial disease, and its effective therapy often demands multiple medications with distinct modes of action. Herein, we report the design and synthesis of multi-targeting novel molecular hybrids comprised of EGCG, a natural polyphenol and quinoxaline derivatives that can effectively inhibit α-glucosidase, α-amylase as well as control oxidative stress by scavenging ROS. Molecular hybrids showed superior inhibition of α-glucosidase along with similar α-amylase inhibition as compared to standard drug, acarbose. Most potent compound, **15c** showed an IC_{50} of 0.50 μM (IC_{50} of acarbose 190 μM) against α-glucosidase and was found to inhibit the enzyme competitively. The binding affinity of **15c** (-9.5 kcal/mol) towards α-glucosidase was significantly higher than acarbose (-7.7 kcal/mol). Compared to vitamin C (IC_{50} 33.04 μM), **15c** exhibited substantially greater antioxidant activity (IC_{50} 18.84 μM). Furthermore, **15c**, with an IC_{50} value of 16.35 μM, effectively inhibited the α-amylase activity. No cytotoxicity was observed for **15c** (up to 40 μM) in MCF-7 cells. Taken together, we report a series of multi-targeting molecular hybrids, representing a breakthrough in the development of effective and novel therapeutic approaches for diabetes.[1]

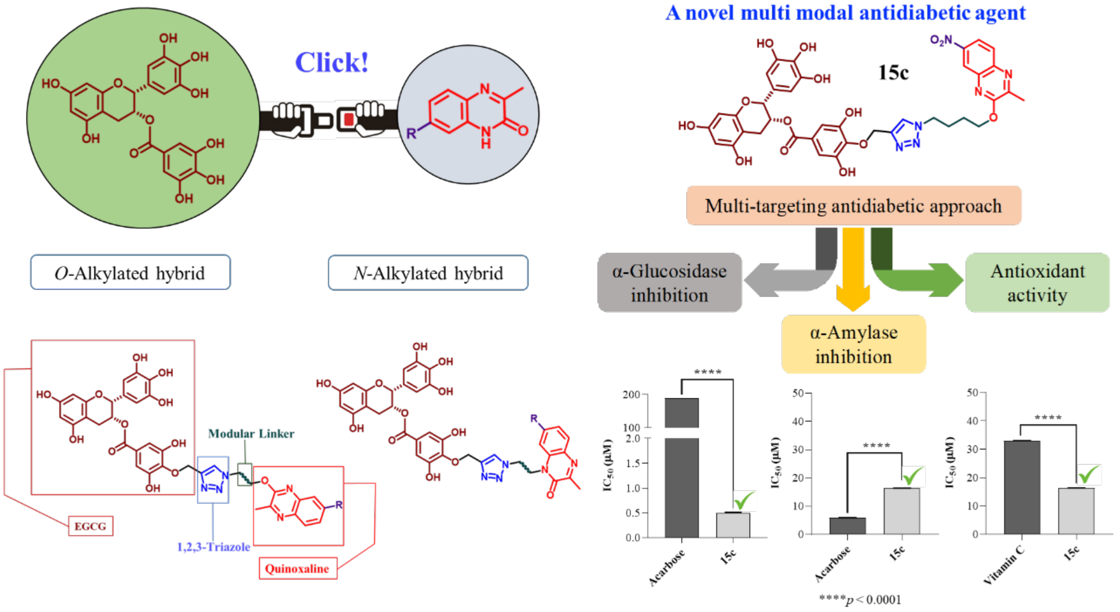

Figure 1. Graphical abstract of natural product-based novel molecular hybrids as multimodal antidiabetics

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Synthesis of Isoxazole Derivatives from Tri-Substituted Donor-Acceptor Nitrocyclopropanes

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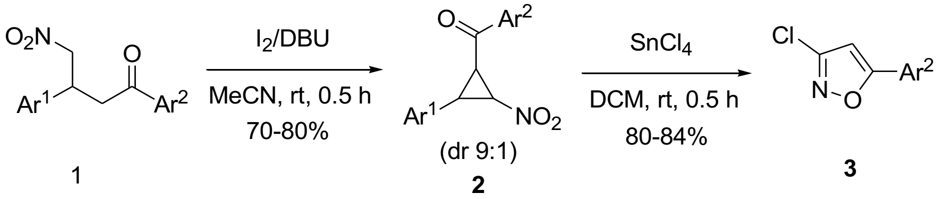
The isoxazole core is frequently encountered in a large number of natural products and synthetic compounds [1]. Isoxazole also serve as versatile synthetic intermediate in organic synthesis. Cyclopropanes have attracted a great deal of attention in organic chemistry owing to their intriguing structural features and unique reactivity. Especially, donor-acceptor cyclopropanes (DACs) have emerged as resourceful building blocks in organic synthesis. When reacted with appropriate reagents, DACs undergo various transformations to yield a plethora of carbo and heterocyclic compounds [2]. In continuation of our interest in DAC chemistry [3], we planned to use Michael adducts **1** for the synthesis of tri-substituted DACs **2** and explore their synthetic applications. Accordingly, when **1** were treated with iodine and DBU in MeCN, they formed a diastereomeric mixture of DACs **2** (~9:1). When cyclopropanes **2** were treated with $SnCl_4$ in DCM, they underwent ring-opening, fragmentation, reduction and cyclization to afford a series of isoxazole derivatives **3** (**Scheme 1**). We will discuss the mechanism of the transformation, substrate scope and further applications in the poster.



Scheme 1

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P-106

Orange Emitting Naphthalene Diimide based Luminogen for Fluorometric detection of Thiol through Click Reaction

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Luminogens with aggregation-induced emission (AIE) are promising for biosensing.[1] Naphthalene diimides (NDIs) are notable for their photophysical properties, electron-deficient core, and ability to self-aggregate through non-covalent interactions.[2] This article outlines the fabrication of an orange-emitting NDI derivative (**NDI-mal**) for fluorometric detection of thiols. Spherical nanoparticles of size 100-150 nm were formed via *J*-type aggregation in a DMSO/DMF-water system. **NDI-mal** exhibited AIE through excimer formation at l_{max} = 588 nm, driven by intramolecular charge transfer from the naphthyl groups to the NDI core.

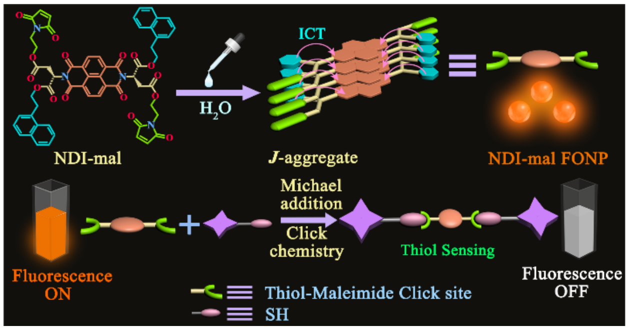

Figure 1. Orange emitting FONPs whose fluorescence intensity become quenched in presence of thiols due to thiol-maleimide adduct formation via Michael addition.

NDI-mal fluorescent organic nanoparticles (FONPs) selectively detected thiols via thiol-maleimide adduct formation, quenching fluorescence with high sensitivity (limits of detection: 15.3 nM for 4-aminothiophenol, 6.0 nM for glutathione, 9.2 ng/mL for reduced BSA) (Figure 1). Thiol sensing was selective and cellular imaging showed that **NDI-mal** FONPs detected cancer cells by quenching fluorescence in B16F10 cells with higher glutathione levels compared to NIH3T3 cells.[3] Fluorescence intensity of native **NDI-mal** FONPs remained in cells undergoing ROS-mediated thiol oxidation through Fenton's reaction. The GSH-maleimide adduct formation exhibited ~2.4-fold higher cancer cell killing through oxidative stress-induced apoptosis, making **NDI-mal** FONPs a selective, sensitive thiol probe with therapeutic potential against cancer cells in absence of systematic intervention.

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P-107

A simple, efficient procedure catalysed for Knoevenagel condensation and Michael addition by organocatalyst.

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Using organocatalyst promotes Michael addition reaction of a variety of α,β-unsaturated alkene (arylidene) compounds, trans-β-nitro styrene with aliphatic and aromatic ketones giving corresponding 1,5-unsaturated products and Knoevenagel condensation reaction of aromatic aldehydes with active methylene compounds affords the corresponding substituted electrophilic alkenes in excellent yields at room temperature within short time. The method is very simple and was monitored by TLC and no further purification was not required. Organocatalyst complexes are prepared from amino acids with metal halides or metal acetates like $NiCl_2$, $Cu(OAc)_2$, $Mn(OAc)_2$, $CdCl_2$, $CuCl_2$, $Mg(OAc)_2$, $HgCl_2$, $Co(OAc)_2$ etc with suitable rection conditions and characterised by EPR, IR , NMR, XRD and UV spectra and ESI mass spectrometer. Moreover, the catalyst has been readily recovered and reused for multiple times without a significant loss of catalytic activity. We try to highlight the applications of the organocatalyst such as copper-thioproline catalyst to different kind of organic carbon-carbon bond formation reactions such as Knoevenagel condensation reaction and Michael addition reaction.

Keywords: Organocatalyst, Knoevenagel condensation reaction & Michael addition reaction, Arylidene, Recyclability.

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P-108

Synthesis of anti-Alzheimer agent taking raltitrexed as a lead

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Protein lysine methyl transferase G9a catalyzes the transfer of the methyl group from S-Adenosyl methionine to the ε-amino group of the selected lysine residue in diversification histone and non-histone substrates such as H3K9, H3K27, H3K56, p53, SIRT1 [1]. G9a controls numerous biological activities such as chromatin remodeling, DNA methylation, proliferation, differentiation, tumor cell movement, apoptosis, and HIV latency [2]. Dysregulation of the G9a has been associated with many diseases like inflammatory disease, neurogenerative disorder, and cancer development. Over the last few decades, considerable inhibitors were reported such as BIX-01294, UNCO224, UNC0321, UNCO638, UNC0642, E72, etc [3]. But they have poor pharmacokinetic properties, clinical utility limitations, and side effects. G9a is a lysine methyltransferase that mainly dimethylates the H3K9 of chromatin, which triggers the repression of genes epigenetically, leading to various diseased conditions, including Alzheimer's disease. Therefore, in order to obtain safer and more potent G9a inhibitors, 3D-QSAR pharmacophore models were engendered based on experimentally known G9a inhibitors. First, we demonstrate that raltitrexed inhibits G9a at 120 nM [4]. Moreover, raltitrexed lowers the total H3K9me2/H3K9 levels in Alzheimer's disease transgenic *C. elegans* CL2006 worms, indicating that raltitrexed targets G9a directly. Since toxicity is the main obstacle to G9a drug development, we evaluated the amount of food that C. elegans consumed and performed thorough in silico toxicity (TOPKAT) evaluations of raltitrexed. This showed that the toxicity or function range of raltitrexed is safe for the worm's growth. Now, as raltitrexed has low BBB permeability so taking raltitrexed as a lead we are synthesizing the new ligands which are designed computationally in discovery studio by best fit we are trying to synthesis an affordable and better drug for Alzheimer's disease G9a / EHMT2 inhibition.

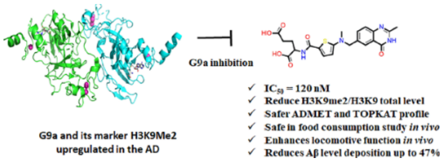

Fig1: graphical abstract of G9a and Raltitrexed

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P-109

Carbonaceous surfaces as drug delivery system: A DFT study

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Carbonaceous nanomaterials, characterized by their ordered nanochannel network and high surface area, play a pivotal role in drug delivery systems. The internal structure, morphology, and surface chemistry of these materials profoundly influence their interaction with drugs.[1] These carbonaceous carriers nanotubes, graphene/graphite, fullerene, and nano-diamonds/diamond-like carbon have garnered extensive attention in drug delivery research due to their highly customizable physicochemical properties and straightforward surface functionalization capabilities.[2] Leveraging their innate hydrophobic nature, these materials exhibit exceptional capability in loading targeted drugs through hydrophobic interactions or π-π stacking mechanisms. This characteristic makes them highly suitable as versatile nanoplatforms for efficient drug delivery. [3]

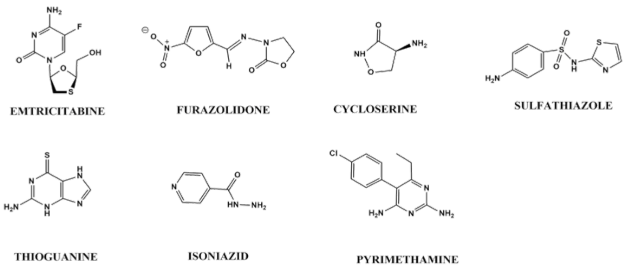

Figure1. Structure of the nitrogen containing drugs interacting with carbonaceous surface

In this study, the interaction between hydrogenated carbonaceous surfaces and nitrogen-containing heteroatom drugs was investigated using Density Functional Theory (DFT). The interaction energies reveal that drug-carbonaceous complexes exhibit stability to a significant extent. Natural Bond Orbital (NBO) analysis indicates an electron transfer from the carbonaceous material to the drug molecule, highlighting a charge redistribution during complex formation. Topological analysis further supports that the interactions involving hydrogenated carbonaceous surfaces and drug molecules are satisfactory. Additionally, quantum mechanical descriptors (QMD) provide insights into the nature of these interactions across all complexes.

The future promise of this study lies on the investigation of the drug and carbonaceous as delivery system with non-hydrogenated surface. These findings can offer a deeper understanding of drug-carbonaceous surface interactions, which may have implications for future drug delivery applications.

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P-110

Development of Lignin-Derived Gold-Titanium Dioxide Nanocomposites for Light Assisted Antimicrobial Photodynamic Therapy

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The overuse of antibiotics has accelerated the rise of antibiotic resistance, creating a critical global health challenge. This issue leads to prolonged hospital stays, increased healthcare costs, and higher mortality rates. Metal and metal oxide nanoparticles (NPs) present a promising alternative, as they interact with essential cellular components like DNA, enzymes, and cell membranes, making them effective antimicrobial agents. In this study, lignin-derived Gold-Titanium dioxide (L@Au-TiO_2) nanocomposites were synthesized and characterized for potential antimicrobial applications. The photodynamic properties of both gold and TiO_2 create a synergistic effect, enhancing their antimicrobial efficacy. Lignin, a renewable and abundant biopolymer, served as a sustainable precursor for nanocomposite synthesis. The structural, morphological, and optical properties of these nanocomposites were thoroughly characterized. Their antimicrobial activity was evaluated against Gram-negative *Escherichia coli*, Gram-positive *Bacillus megaterium*, and the fungal strain *Candida tropicalis* in both light and dark conditions. The results underscore the promising potential of L@Au-TiO_2 nanocomposites in antimicrobial photodynamic therapy, offering innovative solutions in medicine and nanotechnology to address critical biomedical challenges.

Keywords: Lignin, Nanoparticles, L@Au-TiO_2 nanocomposites, antimicrobial, photodynamic therapy

P-111

Band gap and Crystallite size Controlled ZnO Nanoparticles with Al, Zr and Se Dopants for Efficient Visible Light Photo Catalytic Remediation of Food Colorants Polluted Aqueous Systems at 25^0C

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In the family of metal oxides, Zinc Oxide nanoparticles (ZnO nps) are reported to be versatile semiconductor photo catalytic systems possessing tunable physical properties such as band gap and nanoparticle size, as well as cost effectiveness, good recyclability, easy transport and rapid disposability. In recent years, global use of synthetic food colorants has become inevitable in food and confectionary manufacturing and processing industries and their subsequent dispersion into water sources cause severe eco-deadlier effects such as chemical toxicity, genotoxicity, threat to aquatic life systems, non-suitability in agro developmental activities etc. In the present research work, ZnO nps containing selective dopants like Zr in d-block and Al and Se in p-block elements in view of tunable band gap and crystallite nanosizes are chosen as photocatalysts under visible (Solar) irradiations for the degradation of Tartrazine based food colorants in water at 25^0C. ZnO nps with and without dopants are synthesised adopting sol-gel method and are characterised for band gap, nano crystallite size, structure and morphology using UV-DRS, PXRD and FESEM. Visible light photocatalytic activities of doped and undoped ZnO nps for the one pot oxidative degradation of popular food colorants such as Lemon yellow (IH 6597), Apple green (IH 8925), Orange red (IH 7802) and Kesari red (IH 9140) have been chosen and their aquatic degradation kinetics are followed under pseudo-first order conditions. The decrease in the absorbance values at the characteristic λ_{max} values of the food colorants with time intervals are followed by using UV-Vis spectrometer and kinetic parameters are evaluated from the data. The photo catalytic efficiency of catalyst are found out based on the overall rate coefficient values determined in doped and undoped catalysts systems. Additionally, ZnO nps used as photo catalysts are also reported to effectively inactivate gram (+) and gram (-) bacteria contaminants in water. Henceforth, antibacterial activities of the ZnO nps with and without dopants are studied on the inactivation of E.coli gram (-) and S.aureus gram (+) bacteria in aqueous systems, under visible light, aerobic conditions at 25^0C. The results are found encouraging and the use of ZnO nps with and without dopants as potential catalysts appear adoptable. Detailed discussions of the results are put forth in the research paper.

Keywords: Food colorants, solar catalytic degradation, Antibacterial activity, Al, Zr, Se doped ZnO nanoparticles.

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Tunable Reactivity of 2-Alkynylanilines toward *N*-Heterocyclic Compounds Synthesis

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The 2-alkynylaniline moiety has received considerable attention due to their aniline and *o*-alkyne functionalities in a single molecule. These molecules can be easily tuned in a way to synthesize a plethora of *N*-heterocyclic derivatives.[1] These features inspired us to work on it; as depicted in Part A and Part B subsequently.

Part A deals with the merger of two bifunctional moieties, 2-alkynylaniline and alkynylnitriles in the presence of $ZnBr_2$, which offers switchable synthesis of two biologically important motifs; acrylonitrile indoles and 3-cyanoquinolines. The group present on the terminal alkyne of 2-alkynylaniline regulates the reaction pathways, intra- versus intermolecular which thereby adds stereoselectivity and regioselectivity in this protocol (Figure 1, Part A). The conversion of acrylonitrile indole ring to quinoline is an intriguing synthetic utility of this methodology.[2]

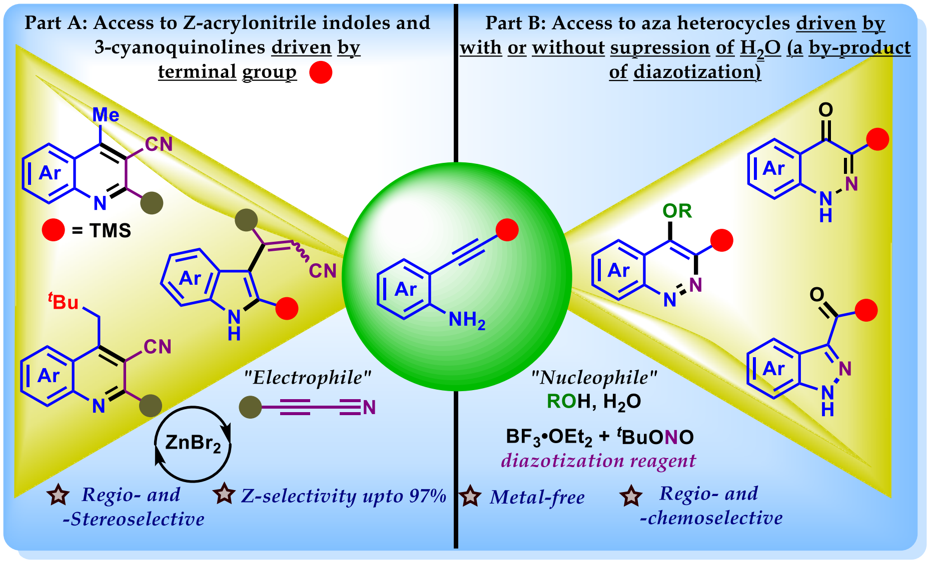

Figure 1. Tunable reactivity of 2-alkynylanilines

Part B deals with a facile and user-friendly protocol for the synthesis of trifluoroethoxy/aryloxy cinnolines, cinnolinones and indazoles from 2-alkynylaniline using metal free diazotization reagent (combination of $BF_3 \cdot OEt_2$ and TBN) in good to excellent yields (Figure 1, Part B). The methodology has been further extended to construct bis-cinnolinones and the chemoselective synthesis of *N*-propargylated cinnolinones.[3]

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P-113

Palladium Catalysis Enabled Sequential C(sp^3)−H/C−C Activation: Access to Vinyl γ-Lactams

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A Pd(II)-catalyzed tandem reaction of aliphatic amides with vinylcyclopropanes has been accomplished by merging C(sp^3)−H and C−C activation. The reaction of VCP revealed alkenylation/cyclization followed by ring opening *via* C−C cleavage, delivering vinyl □-lactams with (*E*)-selectivity. The role of ligands, site-selectivity, functional group diversity, mechanistic insight, and synthetic utilities are important practical features.

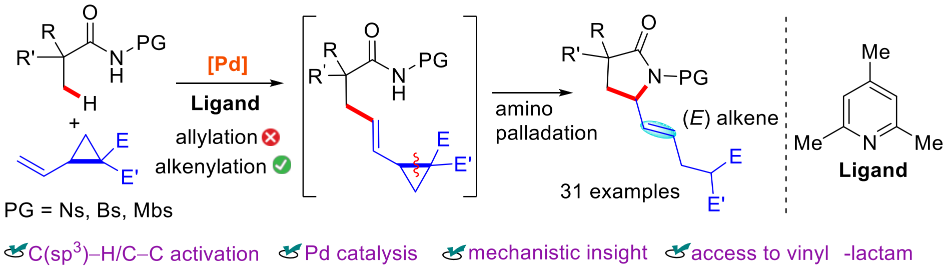

Figure 1. Merging C(sp^3)−H/C−C Activation with VCP

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P-114

Salt-Tolerant, Protease-Stable and Non-Resistance Developing Cationic AMPs for Combatting Planktonic MRSA and its Biofilms

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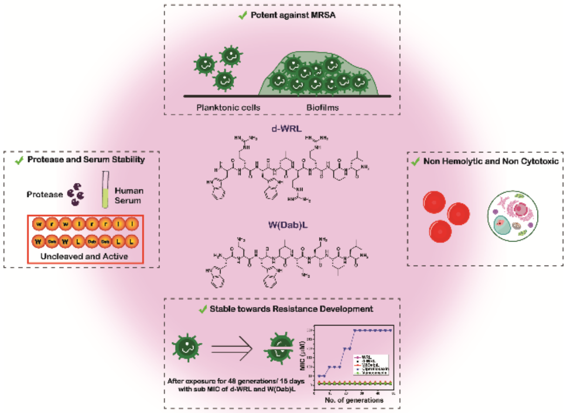
The escalating global antimicrobial resistance crisis necessitates the development of novel therapeutics. Methicillin-resistant Staphylococcus aureus (MRSA), a critical pathogen on the WHO's global list of antibiotic-resistant bacteria, forms biofilms significantly more resistant to antibiotics than planktonic cells. Antimicrobial peptides (AMPs), naturally occurring in organisms across the biosphere, show promise as new treatments. However, their clinical use is limited by high production costs, salt sensitivity, nonspecific toxicity, and protease degradation. In this study, we have developed highly potent, salt-tolerant, non-hemolytic, non-cytotoxic, and proteolytically stable AMPs d-WRL containing D amino acids, and W(Dab)L containing unnatural amino acid 2,4-Diaminobutyric acid that can completely obliterate planktonic forms as well as biofilms of MRSA. We have established that the biofilm eradication potency of d-WRL and W(Dab)L was related to their protease stability. The developed AMPs were membranolytic in their mechanism of action which further led to the absence of development of resistance against it in MRSA for over 96 generations that were studied here, in contrast to conventional antibiotics like Ciprofloxacin. These findings, assessed through various biophysical, spectroscopic, and microscopic techniques, suggested that the developed AMPs d-WRL and W(Dab)L would be a valuable addition to the currently inadequate toolbox of AMPs available for the mitigation of MRSA infections.



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P-115

Synthesis of Sulfur Functionalized Isoindolone Scaffolds from Hydroxyisoindolinones

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An efficient methodology has been developed for the synthesis of sulfur functionalized isoindolone scaffold utilizing *N*-acyliminium ion intermediate of hydroxyisoindolinone, with tosmic and Lewis acid in good to excellent yield. The protocol has been extended for the synthesis of pyrroloisoindolilone derivatives. Furthermore, the methodology also encompasses the synthesis of anticancer intipirdine compounds.

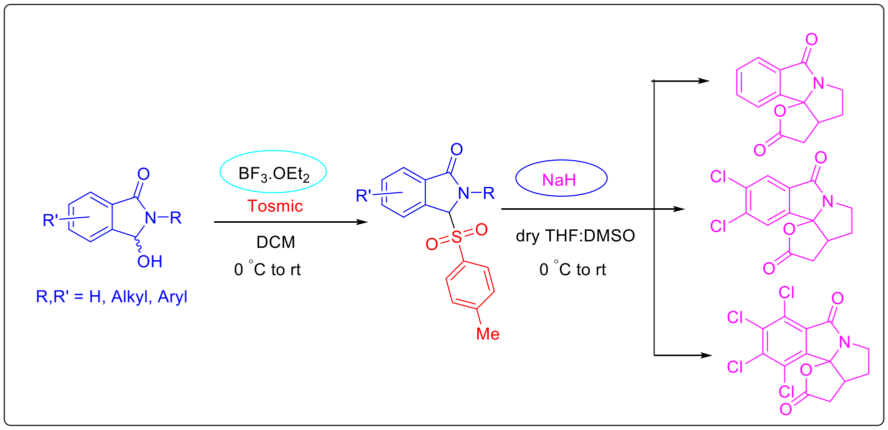

Figure 1. Graphical abstract for the synthesis of sulphur functionalized isoindolone scaffolds

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P-116

Reconstructing Functional Protein from its Fragments

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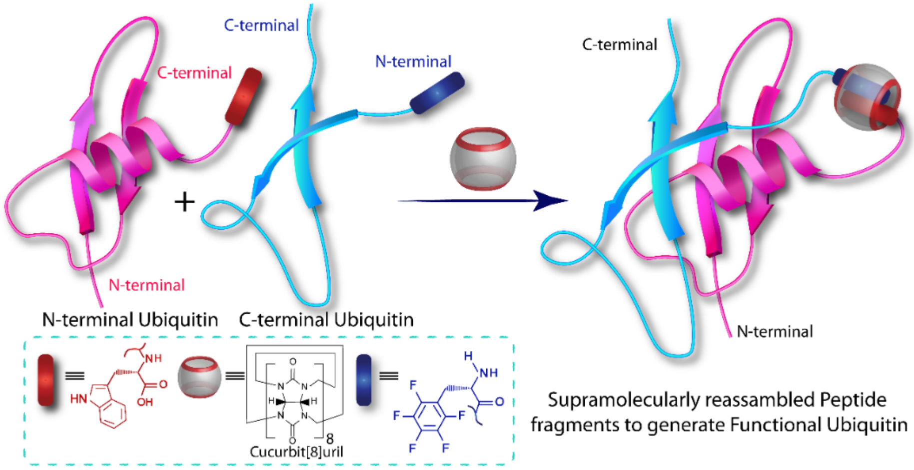
Control over protein function is highly desirable as it will allow us to understand and manipulate the biological phenomenon. In this regard, the Split-Protein Technique (SPT) provides unique opportunities where the fragments of a protein come into proximity and reconstruct the functional proteins.[1] The dissection and subsequent reassembly of a protein from its peptidic fragments allow control over its tertiary structure, and hence its function. In the present work, we utilized the host-guest chemistry of Cucurbit[8]uril (CB[8])[2] to develop a new strategy to reconstruct fully functional proteins from their peptidic fragments. As a proof of concept, two fragments of Ubiquitin are synthesized and functionalized with two guests for CB[8]. Under appropriate conditions, the guests form a ternary complex with CB[8], conjugating the two fragments. The conjugated protein showed similar folding to that of the native Ubiquitin. The activity assay confirmed that the reconstructed protein is fully functional. The observation opens up the possibility of using this newly developed split protein technique for various important biological applications.



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P-117

Tris(aryl)-cyclopropenium-ion Catalysed Bis-vinylation of Aldehydes

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In recent years, the cyclopropenium salts have been explored as organocatalysts in some important organic transformations.[1] Our group has utilized the cyclopropenium based small organic molecules as nucleophilic carbene catalyst,[2] H-bond donor catalyst,[3] Bronsted base catalyst,[4] etc. The bis-vinylation of aldehydes is one of the direct ways to access 1,4-dienes, often referred as skipped dienes. However, there are only two reports available in the literature for this transformation.[5] We envisioned that the cyclopropenium cation could act as an organic Lewis acid catalyst for this transformation. In line with this concept, we have developed both inter- and intramolecular vinylation of substituted aldehydes and the results will be discussed.[6]

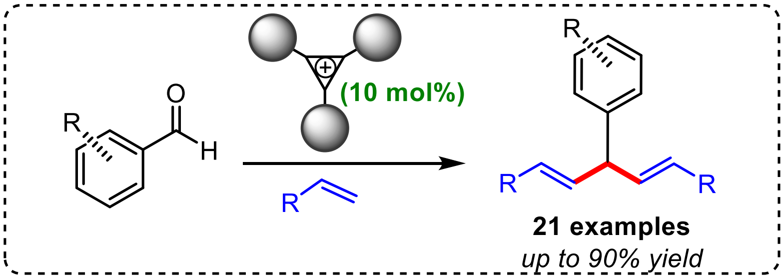

Figure 1. Cyclopropenium ion catalysed bis-vinylation of aldehydes.

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P-118

Ruthenium doped cobalt sulphide electrocatalyst derived from ruthenium-cobalt Prussian blue analogue (RuCo-PBA) for enhanced hydrogen evolution reaction (HER)

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The designing of efficient electrocatalysts for hydrogen generation is essential for the practical application of water-splitting devices.[1] With numerous electrochemical advantages, transition metal sulphides are regarded as the most promising candidates for catalysing the hydrogen evolution reaction (HER) in acidic media.[2] In the present study, Ru doped cobalt sulphide nanosheets termed Co_9S_8/Ru@T (T = 24H, 48H, and 72H) were obtained by varying the reaction time from 24 h to 72 h from a RuCo-PBA precursor.[3] The role of time period for the synthesis of Co_9S_8/Ru@48H is vital in increasing the number of electroactive sites and optimising the hydrogen adsorption-desorption phenomena leading to an increment in the HER activity.

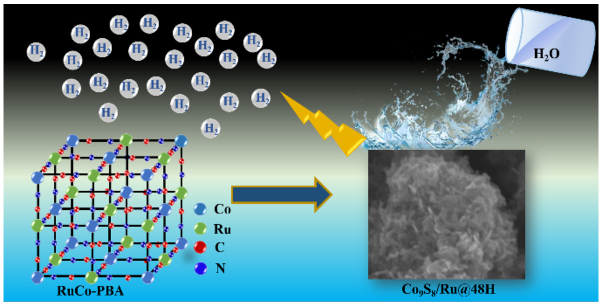

Figure 1. RuCo-PBA derived Co_9S_8/Ru@48H serve as an excellent electrocatalyst for HER.

The electrochemical outcomes demonstrate that the optimized Co_9S_8/Ru@48H requires a low overpotential of just 94 mV to produce a 10 mA cm^{-2} current density, and also possesses a lower Tafel slope value of 84 mV dec^{-1} defining its faster reaction kinetics. The as-synthesized Co_9S_8/Ru@48H was stable up to 20 h of constant electrolysis signifying its outstanding durability. The optimized synthetic approach and impressive electrochemical results make the Co_9S_8/Ru@48H a suitable alternative to noble-metal-based electrocatalyst for HER.

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P-119

Desymmetrization of 2,5-Cyclohexadienones *via* Organocatalyzed Asymmetric Domino Reaction: Direct Entry to the Hydrophenanthren-2(1*H*)-ones

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Hydrophenanthren-2(1*H*)-one is a constitutive unit of a large number of important natural products, including alkaloids, useful lipids and several synthetic bioactive molecules exhibiting a broad range of biological properties.[1] Due to the synthetic and biological relevance of the above-cited core, its stereoselective synthesis is of utmost significance. On the other hand, breaking the plane of symmetry in achiral 4,4-disubstituted 2,5-cyclohexadienones[2] is of huge importance to access not only the interesting scaffolds but also bioactive compounds and natural products.[3] We envisioned that appending another acceptor site at the C-4 position of the 2,5-cyclohexadienones could lead to desymmetrization *via* a domino sequence. While implementing such reactions, control over the formation of several stereocenters and regio-/chemo-selectivity have been perceived as the major challenges. Therefore, a judicious design of substrates and a choice of suitable chiral organocatalysts can expedite regio-/enantioselective addition at the desired positions to create scaffolds with multiple stereogenic centers. For this purpose, we have designed the Michael acceptor-tethered 2,5-cyclohexadienones to undergo a chiral squaramide catalyzed domino 1,4-/1,4-addition sequence leading to desymmetrization of achiral cyclohexadienone unit.[4] Further, we have exploited organic phase-transfer catalysts for the stereoselective 1,6-/1,4-addition sequence with simultaneous desymmetrization reaction between nitroalkanes and 2,5-cyclohexadienone bearing *α*-,*β*-,*γ*-*δ*-unsaturated acceptors.[5] Both processes provided efficient access to tetrahydrophenanthren-2(1*H*)-ones bearing up to five contiguous stereogenic centers in excellent diastereo- (>20:1 dr) and enantioselectivities (up to >99% ee). The detailed findings of our research in this direction will be presented.

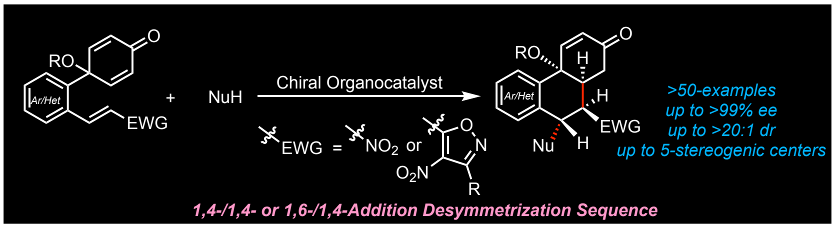

Figure 1. Desymmetrization of 2,5-cyclohexadienones *via* organocatalyzed 1,4-1,4- or 1,6-/1,4-addition reactions

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P-120

Palladium-Catalyzed Weak Chelation-Assisted Site-Selective C-H Arylation of *N*-Aryl Pyridones *via* 2-fold C-H Activation

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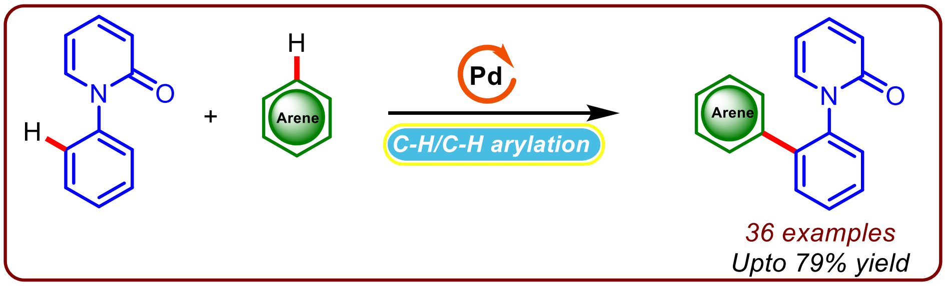
The development of efficient synthetic methodologies for the diversification of pyridone and related heterocycles holds immense synthetic interest as their existence in various natural products and pharmaceuticals. Unlike the structural diversification of the pyridone heterocycle, the method demonstrated here is the arylation of aromatic ring of *N*-aryl pyridone. Accessing the arene C–H bond of *N*-aryl pyridone in the presence of potentially reactive sites on the pyridone ring imposes a formidable synthetic challenge. Herein, we report a Pd-catalyzed site-selective C–H arylation of the *N*-aryl ring with arenes as the aryl source *via* the cross-dehydrogenative coupling utilizing weak chelating pyridone as the directing group.[1] The procedure offers an opportunity to utilize arenes as the coupling partner, obviating the need for prefunctionalized arylation source. The significant features of the method include the use of medicinally important pyridone as the intrinsic directing group, two-fold C-H activation, substrate scope, and late-stage diversification of medicinally important compounds.



✓ ***Pyridone DG*** ✓ ***Arene as aryl source*** ✓ ***Two-fold C-H activation***

✓ ***Site-selectivity*** ✓ ***Broad substrate scope***

Scheme 1. Pyridone directed C-H arylation of *N*-aryl pyridone

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P-121

Design, Synthesis, Computational studies, and evaluation of In-vitro anti-breast cancer potentials of Benzo[d] [1,3] dioxole and 2-Bromofuran tethered 1,2,4 triazole hybrids

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A novel series of seven compounds**,** having Benzo[d] [1,3] dioxole and 2-Bromofuran tethered 1,2,4-triazoles, were designed and synthesized conveniently over four steps with a good yield. Synthesized 1,2,4 triazoles were confirmed by various analytical techniques such as FTIR,^{1}H NMR, ^{13}C NMR, and mass spectrometry. Anti-breast cancer potential was evaluated for the synthesized compounds against MCF-7 and triple-negative 4T1 cell lines. From the results, it was found that compound **12b** showed IC$_{50}$ at 3.41 µg/mL against the MCF-7 cell line, and compound **6a** showed IC$_{50}$ at 3.41 µg/mL against the 4T1 cell line. Further, in-silico studies such as molecular docking to find orientation and binding interaction, ADME prediction to check Lipinski's rule, and molecular dynamics simulation to check ligand-protein stability were carried out.

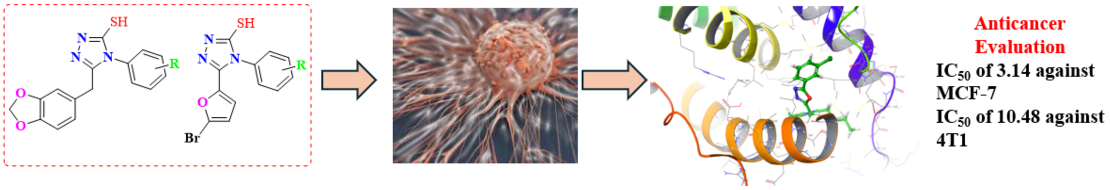

Figure 1. Graphical abstract

Every year, 1.8 million women worldwide are affected by breast cancer, the most frequent cancer in women.[1] Research on anticancer medications is still being done extensively with the goal of developing novel treatments that have lower toxicity and higher efficacy. The five-membered heterocyclic ring triazole is an effective and versatile ring structure and one of the most studied groups of potential chemotherapeutics;[2] here, we report synthesis, characterization, in-silico, and in vitro studies of novel triazole derivatives.

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P-122

Esterase-responsive Self-immolative Prodrugs for the Sustained Delivery of the Anticancer Drug 5-Fluorouracil with Turn-on Fluorescence

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The FDA-approved chemotherapeutic drug 5-Fluorouracil (**5-FU**) is an antineoplastic antimetabolite of the uracil anabolic pathway.[1] **5-FU** has been widely used to treat various types of cancer including lung cancer. It exhibits cytotoxicity by inhibiting the activity of nucleotide synthesizing enzyme thymidylate synthase (TS) to prevent the conversion of deoxyuridylic acid to thymidylic acid in the DNA synthesis pathway.[2] However, **5-FU** possesses some limitations and side effects, such as short half-life, readily converted into inactive form by dihydropyrimidine dehydrogenase (DPD), myelosuppression, central neurotoxicity, gastrointestinal toxicity.[3] To overcome the limitations of **5-FU**, stimuli-responsive prodrugs of **5-FU** are advantageous for the selective delivery of drug to cancer cells with minimized off-target side effects.[4] In the present study, esterase-activatable fluorogenic prodrugs of the chemotherapeutic drug **5-FU** have been rationally designed and synthesized using multi-step organic synthesis. While **5-FU** was connected directly with the fluorophore via a C-N bond in the prodrug **BJ-50**, an additional self-immolative benzylic spacer with a carbonate linker was incorporated in the prodrug **BJ-92**.

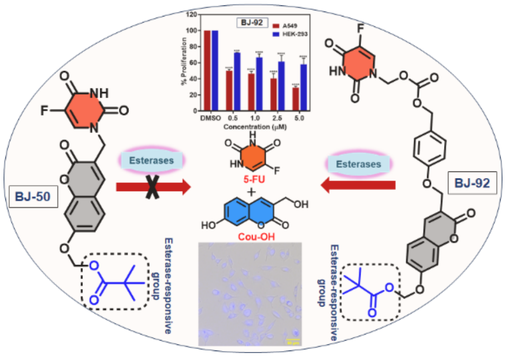

Figure 1. Graphical abstract representing the esterase-responsive activation of prodrugs **BJ-50** and **BJ-92** for the delivery of **5-FU** with turn-on fluorescence.

Although absorption and emission spectroscopic studies revealed the activation of both the prodrugs by porcine liver esterase (PLE), reverse-phase HPLC studies confirmed the inability of **BJ-50** to release the active drug **5-FU**. In contrast, a sustained release of **5-FU** and **Cou-OH** was observed from **BJ-92** in the presence of PLE. The endogenous esterase-mediated activation of the prodrug **BJ-92** was validated by the turn-on fluorescence in A549 cells and the anti-proliferative activities in A549, and HEK-293 cells. Modulation of the expression of a few cancer marker proteins by **BJ-92** and **5-FU** was studied to evaluate their anticancer activities. As esterases are overexpressed in cancer cells, the prodrug in the present study would be helpful in selectively delivering **5-FU** to cancer cells with reduced off-target side-effects.

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P-123

Water-Stable Metal−Organic Framework for Highly Sensitive and Selective Sensing of Metal Ions and Organo-toxin in aqueous Medium with Theoretical Revelation

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Metal−organic frameworks are a class of attractive materials for fluorescent sensing. Improvement of hydrolytic stability, sensitivity, and selectivity of function is the key to advance the application of fluorescent MOFs in aqueous media.[1] In this study, we demonstrated the synthesis of a Zn^{2+} based robust (water and pH =2–12 stable) luminescent microporous MOF, as **1** ($Zn_2(Py)(Atz)_2$ ▪ DMF ▪ $2H_2O$ (H_2Py = 3,5-Pyridinedicarboxylic acid, Hatz =3-Amino-1,2,4-triazole), for the selective sensing of the Fe^{3+} ions and hazardous nitro-explosives (TNP) in an aqueous medium.[2] The sensing of these analytes occurs with remarkable rapidity (~ seconds), and the calculated limits of detection (LOD) for Fe^{3+} ions and TNP are determined to be 22.5 ppb, and 37.7 ppb, respectively. The identification of these analytes was further elucidated through a solid, solution-based, cost-effective paper strip methodology, which demonstrates triphasic identification capabilities. The sensor exhibits reusability without a significant compromise in its detection efficiency. The sensor additionally demonstrated the capacity for recognising Fe^{3+} ions in biological samples, tablets and TNP in river water samples.

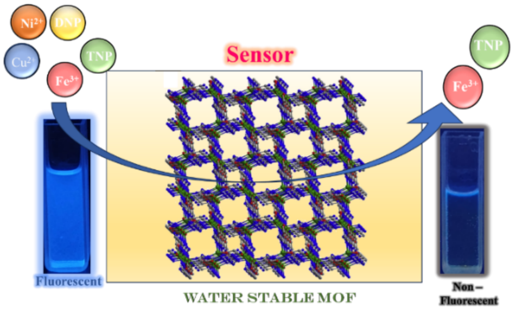

Figure 1. Graphical presentation of detection of Fe^{3+} ions and TNP molecules in water medium.

The sensing merits of **1** motivated us to synthesise a composite of **1**@Gel composite, which manifested colorimetric detection capabilities for these specific analytes. Comprehensive experimental investigations indicated that the mechanisms potentially responsible for the detection of Fe^{3+} ions include photo-induced electron transfer (PET) and fluorescence resonance energy transfer (FRET). This sensing mechanism is additionally corroborated by theoretical study and excited lifetime measurement. The anti-interference ability and recyclability along with the pH stability gave these MOF **1** high potential to be used as practical sensors toward Fe^{3+} ions and TNP in water as a greenest medium.

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P-124

Synthesis and Characterization of Sustainable Zeolite 4A from Kutch Kaolin Clay for Water Remediation: Enhanced by Machine Learning

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The synthesis of synthetic zeolites is tedious, time consuming and costly. To overcome these limitations, we have explored sustainable source of kaolin clay, Kutch for the synthesis of zeolite 4A, via hydrothermal method [1]. Zeolite 4A synthesised was further characterized via, XRD, FE-SEM, FTIR, TGA and BET, which confirms the formation of desired product [2]. Zeolite 4A was evaluated in removing methylene blue dye, below permissible limit. 10 Litres contaminated water with methylene blue was filtered using only 1 gram of zeolite 4A. The experimental data generated was employed for the application of machine learning model for the simulation of equilibrium concentration of the synthesised Zeolite 4A [3]. Gaussian process model was applied which gave satisfactory results having the least objective function value and test error of 0.0148 in stage 1, for the prediction of Ce (Equilibrium concentration), and 3.748e-05 in stage 2, for the prediction of Qe (Adsorption capacity). Overall, the present study highlights the efficiency of raw zeolite 4A and fabricated methodology, for the removal of dye along with incorporating a favourable and robust machine learning model for the simulation of equilibrium concentration.

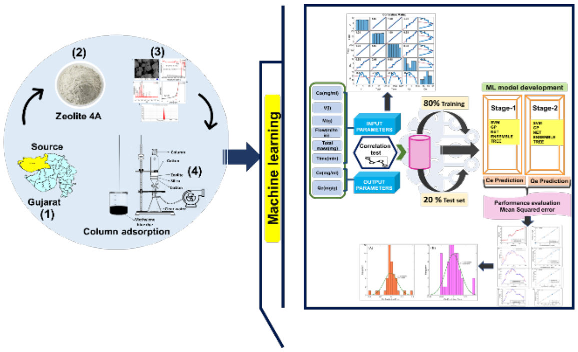

Figure 1. Graphical abstract of the Zeolite 4A utilized for removal of toxic dye and application of machine learning for simulation

First, we synthesized zeolite 4A using kaolin clay of Kutch, to make the whole process cost-effective and eco-friendly. Highly crystalline and porous zeolite 4A was used for water remediation, specifically for the removal of hazardous dye molecule from water, via column adsorption. Machine learning and artificial intelligence plays a major part in prediction of the equilibrium concentration and adsorption capacity of the adsorbent material. The model generated predicts the Ce and Qe with minimum error possible and high accuracy.

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P-125

Construction of Structurally-Complex Multi-Component Coordination Cages

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In the last few decades metal-mediated self-assembly has been widely explored to generate fascinating 2D and 3D architectures from simple building blocks. In this context, Pd(II)-based self-assembled coordination cages possessing 3D cavities are well known for their applications in anionic/neutral guest encapsulation, molecular separation, safe storage for reactive species etc.[1] Among these, coordination cages possessing anisotropic cavities are of great interest as low-symmetry supramolecular hosts due to their close resemblance with the active sites of the metallo-enzymes. The two common strategies explored so far to achieve structurally-complex low-symmetry architectures are: i) integration of more than one type of symmetrical ligands in a single coordination cage (e.g., L^{aa}, $L^{bb,}$ etc.) and ii) utilization of one type of unsymmetrical ligand (e.g., L^{ab}) in the cage assembly.[2] However, controlling the self-assembly process to ensure exclusive formation of a discrete low-symmetry assembly is a considerably challenging task. Further, merging of the above-mentioned approaches to achieve low-symmetry cages equipped with more than one type of unsymmetrical ligand would be even more challenging.

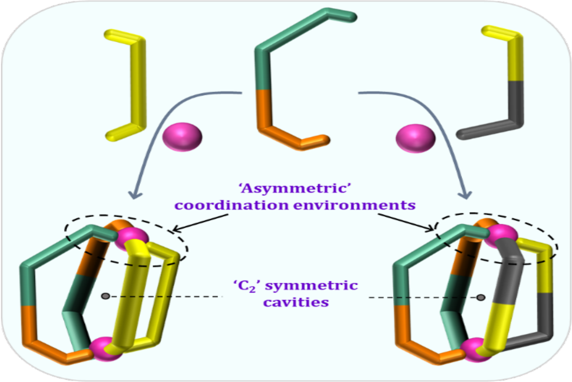

Figure 1. Cartoon representation showing self-assembly of multi-component coordination cages

In this work we have outlined a design strategy for controlled synthesis of highly anisotropic $Pd_2L^{ab}{}_2L^{cc}{}_2$ and $Pd_2L^{ab}{}_2L^{cd}{}_2$-type cages possessing C_2 symmetry cavities through high-fidelity integrative self-sorting of an unsymmetrical ligand with another geometrically complementary symmetrical/unsymmetrical ligand.[3] Structural constraints and geometry complementarity in the ligand design drives the nonstatistical self-assembly of the cages. Both direct ligand assembly and integrative self-sorting of the homoleptic parts resulted in clean formation of the mixed ligated cages. In this study we have also demonstrated a rare heteromeric completive self-sorting process where a fusion of three homoleptic assemblies resulted in simultaneous formation/existence of $Pd_2L^{ab}{}_2L^{cc}{}_2$ and $Pd_2L^{ab}{}_2L^{cd}{}_2$ -type mixed ligated assemblies through cage-to-cage transformations.

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Utilizing Human Calcitonin (hCT) to Prevent the Aggregation of Small Peptide Fragments 0f SARS-COV E-protein: A Computational Approach

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The SARS Corona virus envelope protein is thought to be a key factor in causing respiratory diseases like the common cold, bronchiolitis, and acute respiratory distress syndrome. This protein contains various peptide fragments, including transmembrane, N- and C-terminal regions. Our study focused on 9 residues (TK9) from the C-terminal region, which form β-sheet rich aggregates in solution phase. We investigated the inhibitory effect of human calcitonin on the aggregation of TK9 through Molecular Dynamics (MD) simulations under physiological conditions. Human calcitonin is a 32 amino acid residue polypeptide known for reducing calcium levels and monitoring phosphate levels in blood, and has been used to treat bone-related disorders such as hypercalcemia and Paget's disease.

Our investigation showed that human calcitonin interacts with specific residues crucial for the aggregation of TK9 (TVYVYSRVK), effectively impeding its aggregation. This interaction not only stabilizes the structure of TK9 but also prevents it from forming β-sheets. Furthermore, the presence of hCT leads to an alteration in the secondary structure of TK9, providing further evidence of TK9's stability in the presence of hCT. Through our MD analysis, we unveiled the potential interaction between hCT and TK9, offering insights into the underlying mechanism behind the inhibition of aggregation. These findings shed light on the promising potential of human calcitonin as a therapeutic agent for inhibiting TK9 aggregation.

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P-127

Strategic Disruption and Inhibition of Amyloid Fibrils via Macrocyclic Templated Silver Nanoparticles

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Patients with neurodegenerative disorders encounter significant challenges when fibril formation occurs, as it exacerbates the progression of their conditions. Targeting amyloid fibrils either through inhibition of fibril formation or by disintegration of mature fibrils has attracted considerable research interest[1-2]. A range of supramolecular entities, including cucurbit[7]uril, sulfobutylether β-cyclodextrin (SBE$_7$βCD), and calixarene, have been involved in inhibiting fibril formation. The application of various biomaterials and polymers as coatings on silver nanoparticles has also made significant contributions to the field of fibril inhibition. So, in this aspect, silver nanoparticles decorated with sulfobutylether β-cyclodextrin(AgNPSBE$_7$βCD) were synthesized using wet chemical method. It was successfully characterized using UV-vis, FTIR, TEM and zeta potential. Further, *in vitro* synthesis [3] of insulin fibril in absence and presence of AgNPSBE$_7$βCD was monitored using ThT fluorescence assay, which demonstrates a significant increase in fluorescence intensity of ThT by ~250 fold in absence of AgNPSBE$_7$βCD, indicative of fibril formation. While, in presence of AgNPSBE$_7$βCD, no such change in fluorescence intensity was observed, as shown in Fig1, which points out inhibition of fibril formation. This statement was further supported with TEM images. Incremental addition of AgNPSBE$_7$βCD to the mature fibril solution, leads to the decrease in the fluorescence intensity of ThT, which suggests the disintegration of fibril. When SBE$_7$βCD was used as a coating agent on silver nanoparticles, it demonstrates remarkable efficacy in disintegrating insulin and fibrils into non-toxic, smaller particles, even at minimal concentrations of SBE$_7$βCD. It is worth mentioning that the fibril formation does not takes place at highest concentrations of blank silver nanoparticle. Consequently, silver nanoparticles functionalized with SBE$_7$βCD are poised as exceptionally viable candidates for the disintegration and inhibition of insulin fibrils. This work has been extended to other proteins as well, which are primarily responsible for various other neurodegenerative diseases.

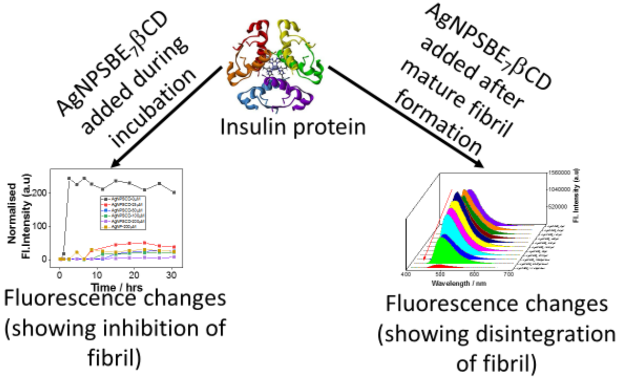

Figure 1. Graphical abstract for the disintegration and inhibition of insulin fibril using AgNPSBE$_7$βCD.

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P-128

A hierarchical porous sheets of bimetallic terephthalate frameworks for sensitive detection of theophylline drug

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Methylxanthines are a group of drugs drawn from innumerable plants and animals. Among this, theophylline (TPH) is an alkaloid drug which was mainly used in the treatment and prevention of a number of respiratory diseases such as asthma and chronic bronchospasm in adults. Unfortunately, it has become a focal point in research due to its narrow therapeutic window and potential side effects making it as a toxic drug when used above its therapeutic range of 10 to 20 mg/mL.[1] To avoid the complications, TPH levels must be carefully recommended. So, electrochemical method plays a significant role in detection of TPH compare to other conventional methods.[2] For this, porous materials received much attention, one such material is metal-organic frameworks (MOFs) also called as porous coordination polymers (PCPs), which are crystalline solids with infinite lattices synthesized from secondary building units (SBUs).[3] These novel hybrids are formed through the strong coordination bond between metal ions or clusters and organic linkers with permanent porosity leading to increased sensitivity towards detection of TPH.

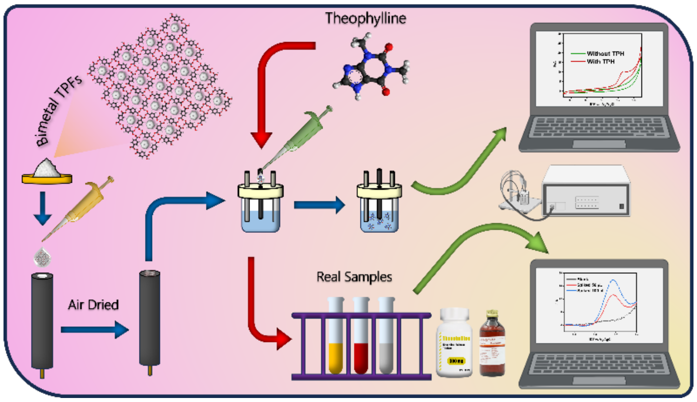

Figure 1. Graphical abstract of the electrochemical detection of TPH.

In this work, a novel bimetal terephthalate framework was synthesized by a facile hydrothermal method and characterized by various microscopic/spectroscopic techniques. Subsequently, the prepared material was casted on the glassy carbon electrode for the amperometric sensing of theophylline (TPH), a drug for various respiratory diseases. The electrochemical experiments were performed with Britton–Robinson (B-R) buffer solution for irreversible electro-oxidation of TPH. The modified sensor shows greater stability, selectivity, reproducibility with low limit of detection (LOD) and limit of quantification (LOQ) of 0.05 μmol L^{-1} and 0.18 μmol L^{-1}, respectively within the linear range of 1.0 x 10^{-6} to 1.50 10^{-4} mol L^{-1} and sensor mechanism was found to be diffusion-controlled phenomena. The proposed sensor offers a promising approach to monitor TPH levels in real-time (synthetic urine samples and TPH tablet and syrups solutions), allowing healthcare providers to adjust dosages and prevent toxicity.

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P-129

Synthesis of $Zn_3V_2O_8$/g-C_3N_4 heterojunction for efficient photocatalytic degradation of water pollutants

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Water pollution is a major environmental issue that poses serious threat to ecosystem and human health. Over the past few years, photocatalysis has gained tremendous attention as a simple and cost-effective alternative for wastewater treatment compared to existing physical and chemical methods. In this study, a novel $Zn_3V_2O_8$/g-C_3N_4 heterojunction was prepared by sonication-mixing method. The formation of heterojunction was confirmed through X-Ray Diffractometer (XRD), Field Emission Scanning Electron Microscope (FESEM), Energy Dispersive X-Ray Spectroscopy (EDX) and UV-visible spectrophotometer (UV-vis). Additionally, the reduction in recombination of electron-hole pair was verified by Photoluminescence (PL) and Time Resolved Photoluminescence (TRPL) spectroscopy. The photocatalytic activity of the prepared samples was investigated through the degradation of congo-red (CR) dye and tetracycline hydrochloride (TC) under visible light. The heterojunction degraded 87.89% CR dye and 79.51 % TC within 120 minutes, with a rate constant faster than that of pure $Zn_3V_2O_8$ and g-C_3N_4. The enhanced photocatalytic activity is attributed to the effective separation of photogenerated charge carriers. Furthermore, the stability of heterojunction was confirmed through three recycling experiments. Thus, we present $Zn_3V_2O_8$/g-C_3N_4 as a promising photocatalyst for degradation of toxic water pollutants.

P-130

Unconventional Supramolecular Assemblies in Metal Organic Multi-component Compounds of Ni(II), Co(II) and Mn(II): Combined Experimental and Theoretical Studies

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Multi-component compounds, which are crystalline materials composed of two or more components (ions, atoms or molecules) in the same crystal lattice, have received remarkable attention in crystal engineering due to the evolving role of solid state chemistry in drug industries, electronic devices and synthetic organic chemistry. It has been firmly established that organic and metal-organic multi-component compounds offer novel solid formulations for active pharmaceutical ingredients, showcasing enhanced features like improved dissolution rates, thermal endurance or mechanical features [1]. Anthraquinone and its substituted derivatives have demonstrated efficacy in crafting coordination compounds, due to their ability to yield compounds with fascinating structural motifs with high thermal adherence topologies [2]. Similarly, coordination compounds of 4-chlorobenzene and substituted derivatives have also attracted immense interest in research fields due to their various potential applications [3,4]. Metal-organic complexes involving cyanopyridines also hold a unique place from a crystal engineering viewpoint [5]. Non-covalent interactions such as hydrogen bonding, halogen bonding, aromatic π-stacking interactions have played many forefront areas of modern chemistry such as materials design and molecular biology [6,7]. However, reports of "charge reverse" halogen bonding, where the electron acceptor halogen atom is located on the electron-rich fragment (anion) and the electron donor atom is on the electron-poor fragment (cation), are still scarce in the literature.

Herein, we have reported the synthesis, crystal structures and characterization of three multi-component coordination compounds of Ni(II), Co(II) and Mn(II), *viz.* $[Ni(3\text{-}CNpy)_2(H_2O)_4]ADS\cdot 2.75H_2O$ (**1**), $[Co(3\text{-}CNpy)_2(H_2O)_4](4\text{-}ClbzSO_3)_2$ (**2**) and $[Mn(phen)_2Cl_2]2\text{-}ClBzH$ (**3**) (where 3-CNpy = 3-cyanopyridine, ADS = anthraquinone-1,5-disulfonate, 4-ClbzSO3 = 4-chlorobenzenesulfonate, phen = 1,10-phenanthroline, 2-ClBzH = 2-chlorobenzoic acid). In compound **1** and **2**, the crystal structure analyses revealed the presence of antiparallel nitrile···nitrile and π-stacked assemblies. In compound **2**, charge reverse Cl···N halogen bonding interactions are observed. The crystal structure analysis of compound **3** revealed the formation of a supramolecular dimer of 2-ClBzH enclathrate within the hexameric host cavity formed. The energetic attributes of the unusual supramolecular assemblies were theoretically examined, employing MEP surface analysis and the computational tools of combined QTAIM/NCI plotting. The remarkable enclathration of the H-bonded 2-ClBzH dimer into the supramolecular cavity were also studied theoretically using density functional theory (DFT) calculations, QTAIM/NCI plotting. Compounds **1** and **2** were subjected to *in vitro* anticancer assessment evaluation in the Dalton's lymphoma (DL) malignant cancer cell line, utilizing the trypan blue assay. Molecular docking was also conducted to investigate the potential interactions of the compounds with anti-apoptotic BCL family proteins.

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P-131

β-Carboline-based light and pH dual stimuli-responsive ion transporters induce cancer cell death

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Stimuli-responsive ion transporters that can be selectively activated inside the cancer cells have shown potential applications as anticancer agents to disrupt ionic homeostasis and trigger cell death. The light and pH dual-responsive ion transporters offer better applicability due to their higher tunability and low cytotoxicity. Herein, we demonstrate thiourea-containing β-carboline-based active ionophores and 4-methyl-3-nitro benzoic acid-linked thiourea-containing β-carboline-based proionophores to facilitate the controlled transport of Cl^- across membranes. The potent compound showed efficient H^+/Cl^- transport activity across the model membranes and cell membranes. Cellular studies revealed that the transmembrane Cl^- transport activity of the potent compound could induce apoptotic and autophagic cancer cell death. The appended photolinker, 4-methyl-3-nitro benzoic acid of the pyridyl ring of the β-carboline moiety, was essential to generate inactive proionophore and improve aqueous solubility. The photoinduced regeneration of active ionophore from proionophore leads to substantial transport of Cl^- across membranes and cancer cell death.

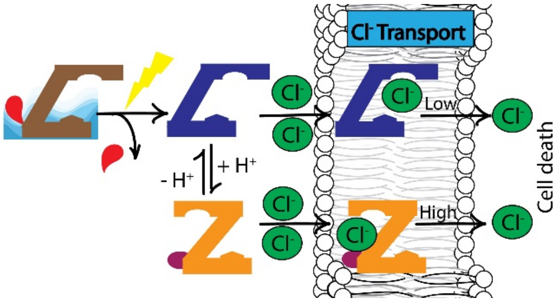

Figure 1. Graphical abstract of dual stimuli responsive ion transporter which causes cancer cell death.

We have developed thiourea-containing β-carboline-based ionophores and a proionophore linked to 4-methyl-3-nitro benzoic acid. Among them, compound **4a** showed selective Cl^- transport across lipid bilayers, with a 1:1 host-guest interaction via a carrier pathway, confirmed by Hill coefficient and U-tube assays. NMR titration revealed interactions of thiourea NH, (Ar)C-H2, and 9H-indolic protons with Cl^-. Mechanistic studies identified H^+/Cl^- cotransport as the main process, which contributes to higher cytotoxicity in cancer cells. The proionophore 5, inactive due to blocked anion binding, becomes active upon photoactivation, leading to Cl^- transport and cancer cell death.

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P-132

Bioinspired Nanoconfinement of Restacked Lamellar Nanofluidic $Ni(OH)_2$ membrane for Enhanced Organic Transformation

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Confinement effect influences biosynthesis, affects protein folding rates, and protects the denaturation of the proteins. [1] Researchers have utilized several nanoconfinement based materials like CNTs, zeolites, MOFs, for the fast transformations of chemical reactions. [2] In this work, we have prepared a lamellar membrane comprising of nickel hydroxide nanosheets grown from the atomic scale by bottom-up strategy. The membrane beholds nanochannels that has been explored for the acceleration of hydroxylation of boronic acids in presence of peroxide. The nanosheets itself enhanced the rate as compared to catalyst free system, which in turn arranging into lamellar stacking hugely accelerated the reaction to several fold. The enhanced basicity inside the nanofluidic channels was found to be the driving factor for the confinement effect. The yield of the product was found to be increased with increase in the channel length and decreased with increase in disorientation of the assembly. The compatibility of the membrane was further studied for various arylboronic acids.

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P-133

Metastable [2]Rotaxane for Selective Fluoride Anion Detection

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A metastable [2]rotaxane is a [2]rotaxane which exhibits kinetic lability in presence of specific stimuli only.[1,2] A [2]rotaxane molecule **2-H·PF₆** is obtained in high yield upon ring-closing-metathesis (RCM) of an acyclic diolefin polyether, in the presence of an axle comprising of anthracenyl moiety and 4-isopropylphenyl slippage stopper (**1-H·PF₆)**. Surprisingly, **2-H·PF₆** exhibited metastability only in presence of fluoride anion, while its topology remained unperturbed in presence of excess amount of the remaining halides such as chloride, bromide and iodide anions.[3] The extrusion of macrocycle 23-crown-7-ether from the [2]rotaxane **2-H·PF₆** was caused by the ion-pair induced deslippage followed by neutralization. The deslippage could be observed in mixed organic-aqueous medium such as acetonitrile-water (98/2). Inorganic fluorides such as potassium fluoride and cesium fluoride afforded sharp fluorescence quenching responses, with the LOD dropping as low as 1.2 x 10^{-7} M. Interference experiments displayed almost complete overlap of the fluorescence responses for fluoride anions in presence and absence of interfering anions. Control study with the corresponding axle **1-H·PF₆** reveals significant fluorescence quenching in presence of all halide anions, thus failing to distinguish between halide anions. Hence, the metastable [2]rotaxane **2-H·PF₆** is well suited for selective and sensitive detection of organic/inorganic species of fluoride ion, in organic as well as organic-aqueous media.

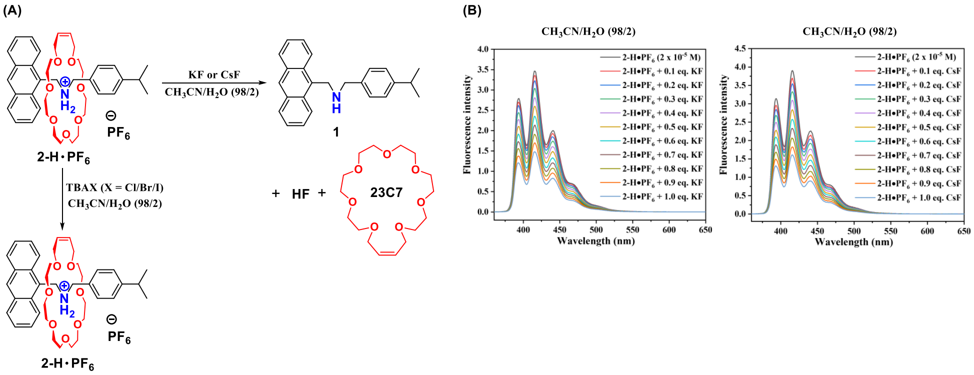

Figure 1. (A) Schematic representation of metastability of [2]rotaxane in presence of fluoride only. (B) Fluorescence quenching response was observed with species such as potassium and cesium fluoride.

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P-134

A Visible-light promoted synthesis of substituted benzo[*c*]-chromeno[4,3,2-*gh*]phenanthridine involving hetero-cross-coupling cyclization and aromatization reaction

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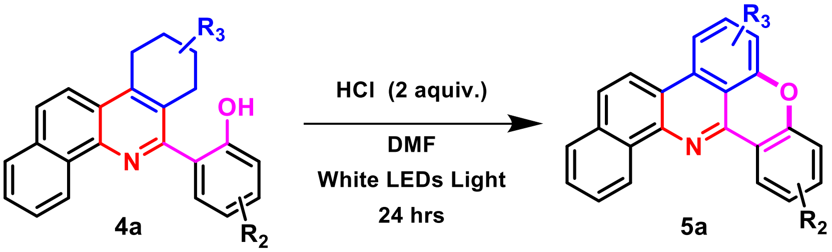
A visible–light–induced radical catalysed synthetic methodology was developed for the synthesis of substituted benzo[*c*]chromeno[4,3,2-*gh*]phenanthridines starting from substituted 2-(7,8,9,10-tetrahydrobenzo[*c*]phenanthridine-6-yl) phenol in DMF as solvent (Scheme 1) and it will be presented. Derivatives of substituted benzo[c]chromeno[4,3,2-*gh*] phenanthridines were obtained by using the inexpensive organic dye eosin yellow as a photocatalyst in a sub stoichiometric amount in presence of 2×9 W white LEDs visible irradiation. A hetero cross-coupling reaction followed by aromatization is taking place in a single step without involving any metal catalyst, or dehydrogenating agent. Notably, 2-(7,8,9,10-tetrahydrobenzo[*c*]phenanthridine-6-yl) phenol derivatives can be easily prepared by multicomponent reaction of commercially available salicylaldehyde, substituted cyclohexanone, and 1-naphthylamine derivatives in a single step.



Scheme 1. Scope of benzo[*c*]chromeno[4,3,2-*gh*]phenanthridine derivatives

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P-135

Deciphering the Antibacterial Action of Bis-Benzimidazole Derivatives through Docking and Molecular Dynamics Simulations on DNA-Topoisomerase-IA

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Bis-benzimidazole derivatives are promising antibacterial agents, exhibiting potential to inhibit DNA-topoisomerase-IA, a key enzyme in bacterial DNA replication. In this study, molecular docking was employed to predict the binding affinities of these derivatives to DNA-topoisomerase-IA. The most potent complexes were further analyzed using molecular dynamics (MD) simulations to evaluate their stability and dynamic behavior over time. Key parameters such as Root Mean Square Deviation (RMSD), Root Mean Square Fluctuation (RMSF), hydrogen bond interactions, and Principal Component Analysis (PCA) were calculated to explore the structural stability and flexibility of the enzyme-ligand complexes. The results revealed that bis-benzimidazole derivatives effectively stabilize the enzyme-ligand complex, showing favorable dynamic properties and strong hydrogen bonding, which contribute to their antibacterial efficacy. This comprehensive analysis provides valuable insights into the mechanism of action of bis-benzimidazole derivatives, highlighting their potential as novel antibacterial agents targeting DNA-topoisomerase-IA.

Keyword: Antibacterial agent, bis-benzimidazole, docking,MD simulation, hydrogen bond.

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P-136

Molecularly imprinted electrochemical sensor based on a metal organic framework-functionalized MWCNTs composite modified electrode for selective uric acid detection

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High level of uric acid (UA) in human body fluid is associated with several medical conditions including gout, arthritis and high blood pressure thus highlighting the need for its regular monitoring to enable early prevention and emphasizing the importance of developing low cost and robust diagnostic tools [1-2]. In this regard, a molecularly imprinted polymer (MIP) based electrochemical sensor has been developed by electropolymerizing polypyrrole (PPy) on the surface of a 3D nanocomposite UiO-66(Zr)-NH-CO-MWCNT modified glassy carbon electrode (GCE) with the addition of UA as the template molecule. The non imprinted electrode (NIP) was prepared in the absence of template UA. The different materials synthesized were characterized by FT-IR, XRD, SEM and the electrocatalytic performance of the sensor was evaluated by using cyclic voltammetry (CV) and differential pulse voltammetry (DPV). CV and DPV analysis demonstrated that the MIP electrode showed enhanced electrocatalytic oxidation of UA. Under the optimized conditions and using the DPV technique, a calibration curve was obtained which gave a linear range from 0.1 to 70 µM and limit of detection (LOD) 0.15µM. The excellent selectivity of the proposed imprinted sensor towards UA was confirmed in the presence of its potential interferents and it was successfully applied to detect UA in real sample matrices with a standard deviation less than 5%. Thus, this work demonstrates the possibility of a new Point of Care Testing (POCT) device for monitoring the uric acid levels in human being.

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Ultra-thin Dielectric Triggered Charge Injection Dynamics for High-Performance Metal Organic Framework/MXene Supercapacitors

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Strategically designed three component heterostructure of MOF-MXene-BN exhibits impressive pseudocapacitive behaviour through a fast charge injection mechanism facilitated by an ultrathin dielectric component, hexagonal boronitride (h-BN). Metal organic framework (MOF), inspite of having higher surface area, suffers from low electronic conductivity, and instability under various operational conditions.

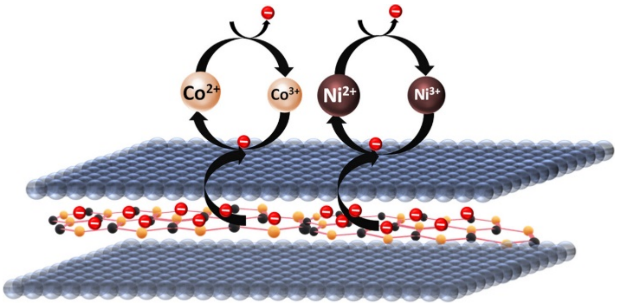

Figure 1. Schematic diagram of the plausible mechanism involving fast charge transfer process through 2D sheets, enhancing electrochemical performance.

Here in we have reported a 2D bimetallic NiCo-MOF, grown over the surface of the exfoliated MXene nanosheets for enhancing the conductivity by providing abundant redox active sites. The issue associated with MXene lies in its tendency to undergo restacking, and can be circumvented by incorporating h-BN between the layers of MXene. Boron nitride serves the dual purpose of preventing restacking and increasing the redox activity across the MXene surface through advantageous charge injection towards the metal ions of the NiCo-MOF. The acquired results were ascribed to synergistically boosted contributions from each participating 2D materials and the formation of a heterostructure (favourable charge injection dynamics) between the MOF, MXene and BN monolayers. Charge transfer mechanisms are elucidated using distribution of relaxation time analysis technique to analyse complex electrochemical impedance spectroscopy data and to differentiate electrode kinetics based on their respective relaxation time constants. The heterostructure of the MOF-MXene-BN delivers a high specific capacity of 942 C/g at 1 A/g and shows an impressive capacity retention of 99.78% over the repeated 5000 charge-discharge cycles. An asymmetric supercapacitor; MOF-MXene-BN//activated carbon achieves a specific capacity of 798 C/g, an energy density of 81 Wh/kg at 365 W/kg, and 81% capacitance retention over 5,000 cycles.

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P-138

Theoretical Investigation on Atmospheric Fate of $CH_3CH_2C(O)OCH(O)CH_3$ Radical

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It is well established that the fluorinated esters (FESs) are the primary products of the atmospheric oxidation of hydrofluoroethers (HFEs).[1-3] For example, $CF_3C(O)OCH_2CF_3$, 2,2,2-trifluoroethyl trifluoroacetate (TFETFA) can be produced from the OH radicals and Cl atoms initiated oxidation of $CF_3CH_2OCH_2CF_3$ (HFE-356mf-f) in the atmosphere.[7] Like HFEs, FESs also undergoes photochemical oxidation in troposphere with atmospheric oxidants, OH radicals or Cl atoms in marine environment. The degradation of FESs produce environmentally burdened product like trifluoroacetic acid (TFA) and COF_2. A detailed quantum chemical study is performed on the unimolecular decomposition reaction of the alkoxy radical, $CH_3CH_2C(O)OCH(O)CH_3$ produced from $CH_3CH_2C(O)OCH_2CH_3$, ethyl proponoate at M06-2X level of theory using 6-31+G(d,p) basis set. Five plausible decomposition pathways including alpha-ester rearrangement, reaction with O_2 and thermal decomposition (C –C, C –H and C –O bond scissions) have been considered in detail. Out of the five prominent decomposition channels, our results reveals that α-ester rearrangement is the dominant path for the decomposition of $CH_3CH_2C(O)OCH(O)CH_3$ radical in the atmosphere involving the lowest energy barrier.

Keywords: Alkoxy radical, DFT, IRC calculation, Rate constant

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P-139

Synergetic Combination of Bio-Electrolytes and Bio-Fluidic Channels as a Novel Resource of Sustainable Energy

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Exploration for sustainable energy resources is essential to minimize our dependence on fossil fuels and to improve environmental parameters. Here, we examined the possibility of utilizing bio-waste-derived electrolytes as an electrical energy resource by placing them across semipermeable membranes prepared through parallel stacking of coir fibres. The nanofluidic membrane (d-CF-V) prepared by modifying the inner walls of the bio-fluidic channels with atomically thin layers of vanadium pentoxide (VO) showed excellent perm-selectivity ($t_+ = 0.87$, with 1000-fold concentration difference) and electricity conversion efficiency (~ 28.2 %). With simulated sea and river water, the d-CF-V yielded output energy up to 2.4 W/m^2, similarly with mineral acid bases (0.5 M HCl and 0.01 M NaOH), the d-CF-V showed an energy output of 11.8 W/m^2. The sun-dried *Garcinia morella* (Kuji thekera), and charred peels of *Musa balbisiana* (banana) were used as sustainable sources of bio-electrolytes, which in combination with permselective d-CF-V yielded a power density of about 1.4 W/m^2. By replacing standard Ag/AgCl electrodes with nanomaterials exhibiting contrasting charge transfer activities, oxidized carbon nanotube membrane (o-CNT) and polyaniline (PANI) membrane the output voltage was enhanced from - 127 mV to - 568 mV, and current output was increased from 10.2 μA to 51.5 μA.

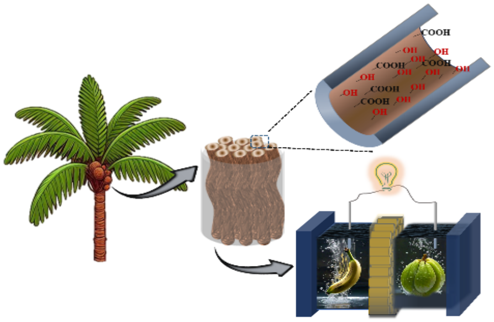

Figure 1. Osmotic energy harvesting using d-CF-V membrane using natural acid and base as electrolytes.

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P-140

Manganese empowered covalent organic polymer composite: Innovative Composite Materials for Next-Generation Energy Storage

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The rising popularity of organic materials in energy storage applications, particularly as electrode materials for supercapacitors, has been notable.[1] Despite their competitive performance, challenges such as morphology distortion and rapid capacity fade have impeded their overall battery performance. To address these issues, researchers have shifted their focus towards organic based composite materials.[2] This study explores the development of sodium iodide decorated manganese doped covalent organic polymer (COP) composite materials as advanced electrode materials for supercapacitors. COP and manganese act a rugged base material with strength and high porosity contributing to the physical and mechanical properties, whereas the sodium and iodine takes part in electrochemical activity. The semi crystalline structure of the composite material was confirmed by X-Ray Diffraction (XRD)[3] where and Scanning Electron Microscopy (SEM) analysis showed nano ball like morphological characteristics. Electrochemical tests, including cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS), demonstrated high specific capacitance of 68.2 F/g, excellent rate capability, and robust cycle stability, attributing to the synergistic effect of the COP matrix and the composite architecture. These results indicate that COP composites are promising candidates for high-performance supercapacitor electrodes, offering an effective route to improving energy storage systems.

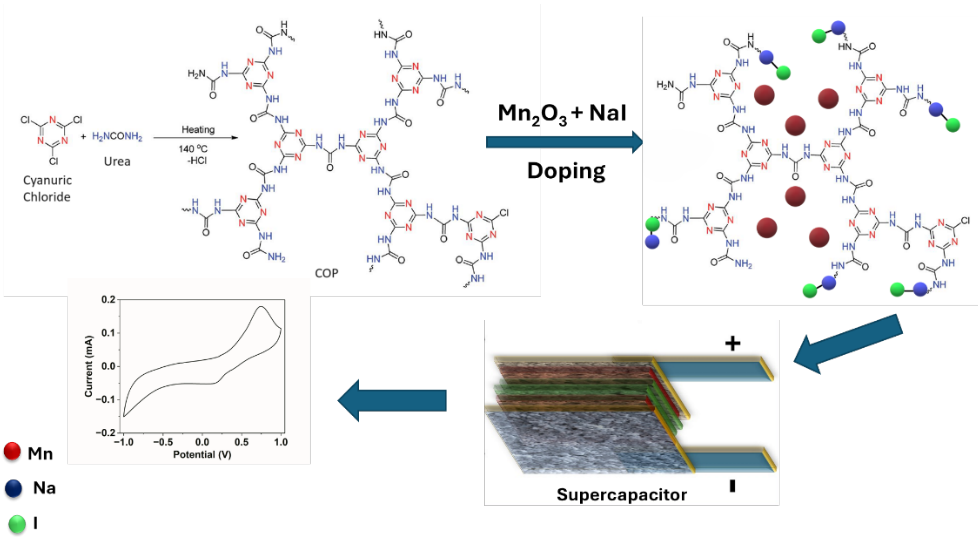

Figure 1. Synthesis of COP/Mn/NaI composite and use as electrode material for supercapacitor and its electrochemical activity

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P-141

Nano-size zirconium oxide as an efficient adsorbent and a photocatalyst in visible light

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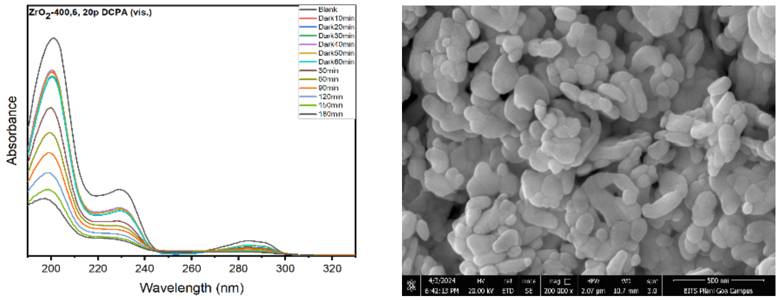
ZrO_2 is a well-established pharmaceutical and ceramic material due to its stability in extreme conditions, biocompatibility, mechanical strength, and non-corrosive nature. [1] As an excellent support material and lone catalyst, it has efficiently catalyzed the formation of economically essential compounds, such as biodiesel, methanol, etc., from hazardous gases. [2] Another potential it holds is as an optically active material amassing application as an optoelectronic device, fuel-cells etc. However, its use as a photocatalyst is limited because of its wider band-gap (~5.25 eV) [3] that restricts activity in UV-region, let alone in visible.



(A) **(B)**

Figure 1. (A) Degradation profile of a pesticide with ZrO_2 in visible region (B) FESEM images of prepared ZrO_2

In our current research work, ZrO_2 nanoparticles are synthesized by the co-precipitation method. X-ray diffraction technique and Raman spectroscopy characterized the resulting material, which confirmed the coexistence of the monoclinic and tetragonal phases. TEM image analysis gave an average particle size ranging from 30nm-70nm, which aligns well with particle size superficially taken from FESEM images. Surface properties like BET were studied to analyse the material's specific surface area and pore volume, and XPS was checked for the existence of oxygen vacancies. Optical properties were studied to know the band-gap of the current material and dynamics of electron-hole recombination in the incident light to gauge its suitability as a photocatalyst.

A complete photodegradation of a pesticide was observed in the UV region and an effective 75% photodegradation in the visible region in 3 hours. Photodegradation with established photocatalyst like ZnO and TiO_2 was considered in visible light to compare its photo efficiency with the current material's. As a metal-oxide-based photocatalyst, it showed tremendous stability and photocatalysis up to multiple cycles.

ZrO_2 prepared with the current method possessed relatively excellent pesticide adsorption within 5 minutes in the dark and active photodegradation afterward, indicating no inactivation of the catalyst's surface after adsorption for subsequent photodegradation reactions. [4]

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P-142

One pot Metal-free synthesis of Aryl Fluorenones

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Fluoren-9-one and its derivatives are privileged structural scaffold which constitute the core of diverse array of compounds exhibiting amazing biological and pharmaceutical activities.[1] Owing to their interesting spectrophotometric properties like intense blue photo- and electroluminescence, liquid crystalline properties, etc.; these classes of compounds find considerable attention among the physical-organic chemists, photochemists as well as material scientists.[2] The known synthesis of aryl fluorenones involve the transition metal mediated multiple arylation steps. Inspired by the previous reports from our group,[3] we have developed an unprecedented highly stereo and regioselective multi component reaction involving an aryl aldehyde, an amine, and Meldrum's acid to produce a new class of hydroquinolines decorated with three stereocenters. This reaction was then utilized for the Metal free one pot synthesis of hydrofluorenones and aryl fluorenones.

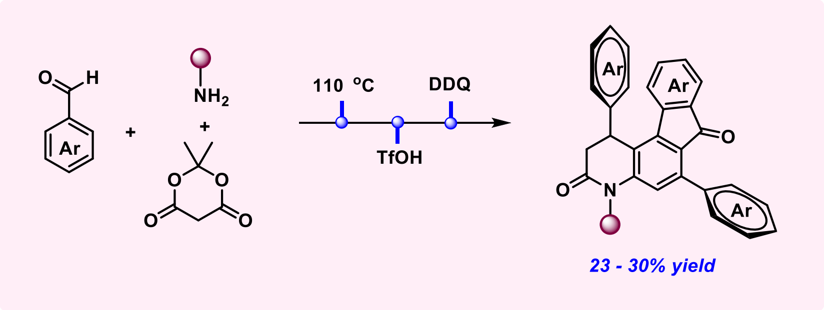

Figure 1. One pot Metal-free synthesis of Aryl Fluorenones.

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P-143

Extraction, isolation and characterization of pure compound from the leaf of the Phlogacanthus thyrsiformis

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Phlogacanthus thyrsifomis is a flowering and edible plant locally called as Nongmangkha in Manipur belongs to family Acanthaceae. Traditionally, it is used as a food items like suktani, dry cooking and it is also a well known medicinal plant used for treatment of many diseases like cough, fever, intestinal disorder, gastritis, pharyngitis, asthma, diabetes etc. *Phlogacanthus thyrsiformis* is an evergreen shrub which has been known to possess antibacterial, anti-diabetic, anti-inflammatory, anti-cancerous and hepatoprotective activity. Various parts of the *Phlogacanthus thyrsiformis* plant has been reported to use as antiseptic, insecticide and as an anti-allergic. Some of the compound has been isolation and identification including new butenoliode, a lactone glucoside and three known compounds identified as sitosterol, lupeol and betulin that were already reported to be present in the leaves of the *P.Thyrsiflorus* but their complete characterization using X-ray crystallography is not reported. Here, we report a pure compound isolated from *Phlogacanthus thyrsifomis* and its characterization carried out by using Spectroscopic technique. The single crystal structure of the solvate compound (1S, 4aS, 5R, 8aS)-1, 4a-dimethyl-6-methylene-5-(2-(5-oxotetrahydrofuran-3-yl)ethyl)decahydronaphthalene-1-carboxylic acid was studied

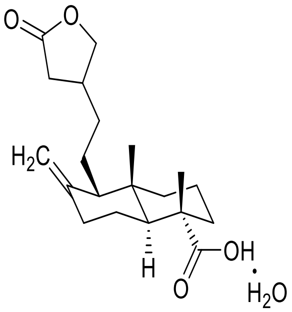

Figure 1: Solvate of (1*S*,4a*S*,5*R*,8a*S*)-1,4a-dimethyl-6-methylene-5-(2-(5-oxotetrahydrofuran-3-yl)ethyl)decahydronaphthalene-1-carboxylic acid

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TYPE-C silica-hydride columns can perform ANP, RP and ONP and Adenine nucleotides separated in UDA (Undecanoic acid) Chemistry by HPLC-RP Method

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Silica-hydride technology offers a considerable advance in HPLC column technology. TYPE-C silica consists of high purity, low metal content silica particles that have been manufactured so that their surface layer is populated with silicon hydride (Si-H) instead of silanols (Si-OH). These phases are formed from a high purity Type B silica backbone, by replacing >95% of the surface silanols with Si-H. It can be seen that the internal structure of silica-hydride and 'ordinary' silica is essentially the same, in that the siloxane bonds leading to rigidity and strength are the same. The difference is that the surface silanols are replaced with Si-H, which create a stable hydrophobic surface. The lack of silanols on the surface also means that end cappingis not required.

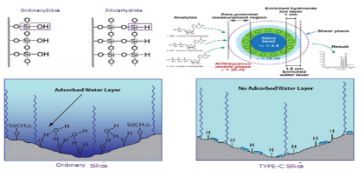
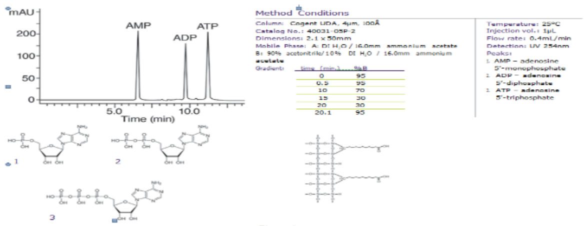


Figure 1



Method Conditions

Column: Cogent UDA, 4µm, 100Å
Catalog No.: 40031-05P-2
Dimensions: 2.1 x 50mm
Mobile Phase: A: DI H_2O / 16.0mm ammonium acetate
B: 90% acetonitrile/10% DI H_2O / 16.0mm ammonium acetate
Gradient:

time (min.)	%B
0	95
0.5	95
10	70
15	30
20	30
20.1	95

Temperature: 25°C
Injection vol.: 1µL
Flow rate: 0.4mL/min
Detection: UV 254nm
Peaks:
1. AMP – adenosine 5'-monophosphate
1. ADP – adenosine 5'-diphosphate
1. ATP – adenosine 5'-triphosphate

Figure 2

Figure 1. Type C Silica Comparison with Type B Silica ; **Figure 2**. Undecanoic Acid (wcx)

UDA is a unique selectivity phase in which the silica-hydride surface is bonded, via a double attachment, to an eleven carbon chain terminating in a carboxylic acid (undecanoic acid). This gives the phase weak cation-exchange properties in addition toaqueous normal-phase. The terminal carboxylic acid group contributes some additional selectivity to the phase which can be useful for closely related compounds. When the mobile phase pH is greater than 5.9, the acid group becomes 90% negatively charged and at pH 6.9 it is 99% charged,and so it may act as a cation-exchanger. Below pH 4.9 the group does not have significant ion-exchange properties. Cogent UDA is a good choice for scientists working with closely related compounds and with LC-MS. Precise methods are easily developed, even with complex sample matrices, with very little desalting required.

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P-145

Piezoelectric Nanomaterials for Ultrasound-Mediated Therapy

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Piezoelectric nanoparticles have emerged as the new generation material for ultrasound (US) based therapeutic applications. With the advent of high penetration depth and non-invasive nature, ultrasound offers various therapies such as generation of reactive oxygen species (ROS) at the intra/extracellular space in remote areas of body, stimulation of neurons in brain tissues, tumor ablation, and antimicrobial activity. However, such applications are limited due to large size of the piezoelectric nanomaterials which substantially reduces cellular uptake and subsequent therapy. With the ability to synthesize highly colloidally stable < 100 nm piezoelectric nanoparticles, we have been able to perform several cell based therapy suitable for neurodegenerative diseases, targeted cancer cell therapy.

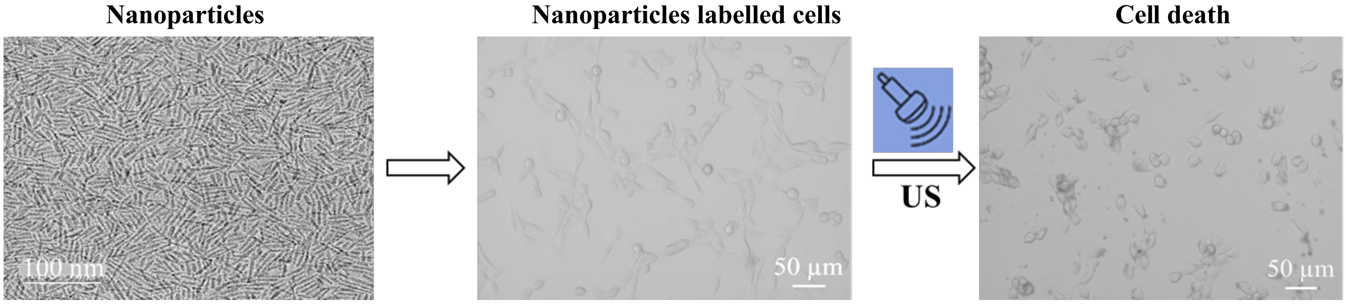

Figure 1: Under ultrasonic exposure piezoelectric barium titanate nanorod that produce ROS inside cell

For that purpose, we have synthesized various piezoelectric nanoparticles like barium titanate (BTO) nanorod[1], calcium phosphate nanorod, lysosomal fibrils and have studied their piezoelectric properties in presence of ultrasound. By modifying the surface of BTO, we can selectively target cancer cells and by generating reactive oxygen species, apoptosis can be induced. For calcium phosphate nanoparticles, to enhance its piezoelectricity and cellular uptake we have conjugated it with gold nanoparticles. Besides, we report a piezoelectric hydroxyapatite nanowire-embedded poly-(vinylidene fluoride) (PVDF) film for ultrasonic electroporation-based delivery of foreign materials to adherent cells. This embedment enhances the piezoelectricity by 3 times.[3] In our work, we used folate/dopamine/arginine functionalised BTO nanoparticle to target cancer cell selectively for inducing autophagy or apoptosis. As an apoptosis marker, we have quantified the expression of different proteins like caspase, Bcl 2 etc. In another work, we have functionalised it with arginine molecule as it helps in direct uptake.[2]By varying the dose of ultrasound, we can regulate autophagy vs apoptosis.

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P-146

A Thiophene Functionalized Hf(IV) Organic Framework for the Detection of Anti-Neoplastic Drug Flutamide and Catalysis of Friedel-Crafts Alkylation

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The advance growth of anticancer drugs characterizes a capable strategy in targeted cancer therapy for improving the selectivity, efficiency and stability of active compounds. The rapid detection and quantification of antibiotic and anticancer drugs in biological samples with fast and sensitive methods is a crucial task for the operative monitoring of drug therapy. The present work describes the design of a porous metal-organic framework (**1**) between Hf(IV) and 2-(thiophene-2-carboxamido)terephthalic acid linker (surface area = 571 m^2 g^{-1}). Desolvated **1′** displayed highly discriminative fluorescence sensing (turn-off response) property for the anti-neoplastic drug flutamide in an aqueous medium even in the presence of co-exiting biomolecules and ions, for the first time. Material **1′** demonstrated a very quick response for the fluorometric detection of flutamide in an aqueous medium. The MOFs response time for sensing flutamide was less than 5 s. This response time along with the probe's exceptionally low detection limit 1.5 nM demonstrate the probe's exceptional capacity to sense flutamide. With a consistent sensing ability, the MOF probe also demonstrated notable recyclability up to five cycles. The probe also displayed outstanding sensing capabilities for flutamide in different pH media, a variety of real water samples and different biological fluids. Density functional theory (DFT)-based calculations were computed to examine sensing mechanism of flutamide with the MOF. Different experimental methods and theoretical calculations unraveled that photoinduced electron transfer (PET) in the presence of flutamide are most likely reasons behind the fluorescence quenching of MOF. Besides the superior activity of **1′** in the sensing application, its catalytic performance was examined in the Friedel-Crafts alkylation reaction between indole and β-nitrostyrene under mild experimental conditions. The observed catalytic data indicated that **1′** is highly promising solid to provide 96% yield and four times usable with a slight decay in its activity. The enhanced activity of **1′** is due to the functionalized thiophene moieties through hydrogen bond donating sites, confirmed by series of control experiments.

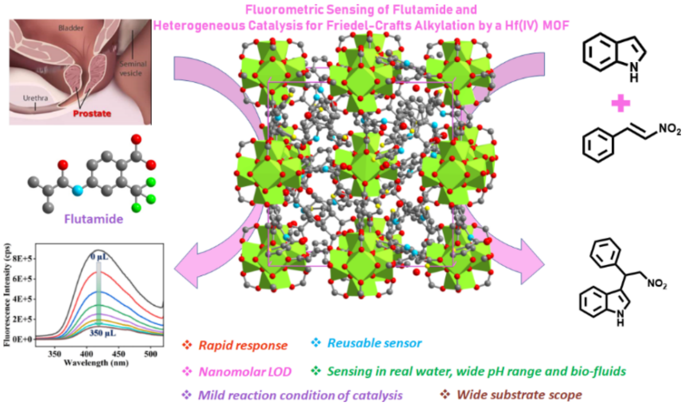

Figure 1. Details of the sensing of anti-neoplastic drug flutamide and heterogeneous catalysis for Friedel-Crafts Alkylation by **1′.**

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P-147

Formation of Bis-indolylmethanes from Symmetrical Triarylmethanes via Brønsted Acid Catalyzed C–C Bond Breaking Reaction

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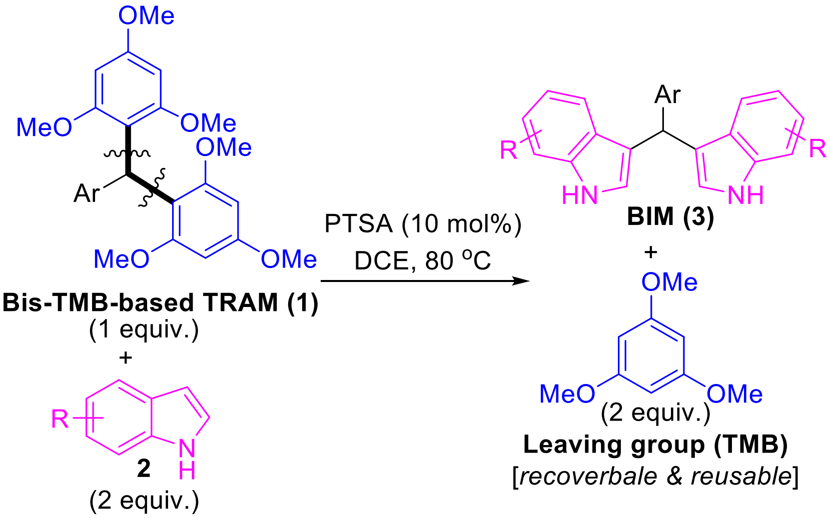
The C–C bond-breaking reactions are very much familiar in biological systems whereas the utilization of carbon-based leaving groups to succeed in C–C bond-cleaving reactions is still underexplored in the field of organic synthesis. An alternative approach to synthesize bis-indolylmethanes (BIM) *via* a unique *p*-toluenesulfonic acid (PTSA) catalyzed dual C_{sp3}–C_{sp2} bond breaking reaction has been reported (**Scheme 1**). In the reported protocol, 1,3,5-trimethoxybenzene (TMB), an electron-rich and sterically bulky arene, acts as a carbon-based leaving group which can be recovered after the completion of the reaction. In this process, several BIMs of various indole derivatives can be synthesized from symmetrical triarylmethanes (TRAMs) containing bis-TMB motifs. By modifying the reaction conditions, we could control the sequential bond cleavage of two C_{sp3}–C_{sp2} bonds in starting TRAM.



Scheme 1. PTSA catalyzed dual C–C bond cleaving reaction in TRAM **1**.

P-148

Unveiling Hetero Atom Containing Fluorescent Carbon Dots from Indigenous Soil Bacterial Metabolites for Toxic Cr (VI) Ion Detection

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Bacteria and its metabolites can be a promising source for the synthesis of fluorescent Carbon dots. The liquid containing the metabolites (organic acids, fatty acids, proteinaceous substances) produced by microbial growth and remaining nutrients is called the cell-free supernatant. In this work, we have explored the potential of indigenous soil bacteria for the synthesis of carbon dots and their application in heavy metal detection in water. We have isolated a bacterial strain, and successfully synthesized fluorescent carbon dots through hydrothermal treatment of the cell free supernatant of the bacterial culture. The formation of carbon dots was characterized by fluorescence spectroscopy, uv-vis spectroscopy, FTIR, FETEM, zeta potential etc. The synthesized carbon dots exhibited strong fluorescence and expectational stability under various conditions. They unveiled the presence of hetero atoms like Nitrogen and Sulphur on their surface. The carbon dots acted as a potential nanosensor for the detection of Cr (VI) even in real water samples demonstrating strong fluorescence quenching in seconds with a limit of detection of about 30 nM. The carbon dots were screened through a number of plausible coexisting analytes that exhibited impressive selectivity towards Cr (VI).

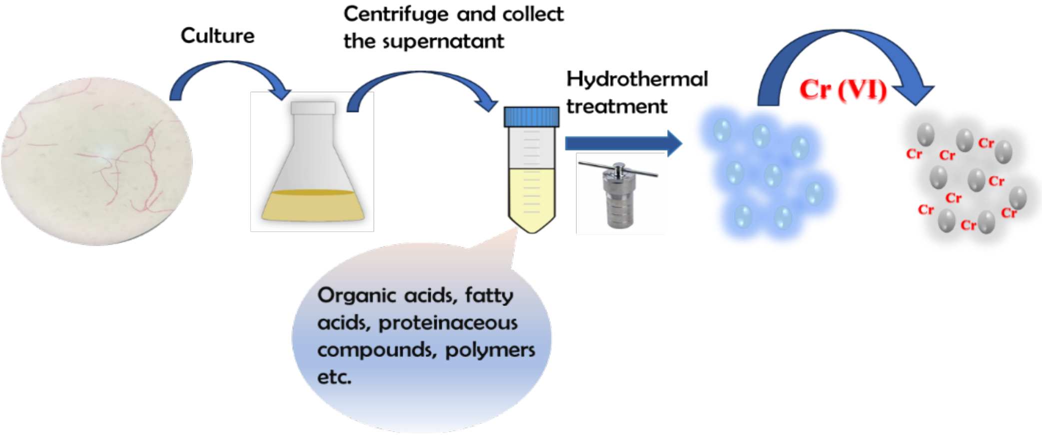

Figure 1. Green synthesis of carbon dots from bacterial metabolites via hydrothermal method for Cr (VI) detection.

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P-149

White Light Emission from Zn(II) and DMSO-Induced Copper Nanocluster Assembly

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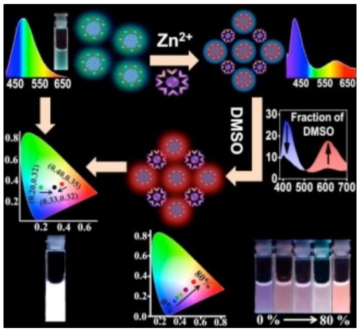
An assembly of metal nanoclusters driven by surface ligands and solvent environment may engender entirely new photoluminescence (PL). Herein, we first synthesize histidine (His) stabilized copper nanoparticles (CuNPs) and, subsequently, copper nanoclusters (CuNCs) from it using 3-mercaptopropionic acid (MPA) as an etchant. The CuNCs originally emit bluish-green (λem=470 nm) PL with a low quantum yield (QY∼1.8%). However, it transformed into a dual-emissive nanocluster assembly (Zn-CuNCs) in the presence of Zn(II) salt, having a distinct blue emission band (λem = 420 nm) and a red emission band (λem = 615 nm) with eight times QY (∼9.1%) enhancement. The temperature dependent emission spectra of Zn-CuNCs depicted that the blue emission originates from the locally excited state (LES) emission of the nanoclusters, while the red emission originates from through-space interaction (TSI) within the assembly. Adding dimethyl sulfoxide (DMSO) further modifies the emission intensities; the red band was amplified four times, while the blue band was diminished by 2.5 times. The transmission electron microscopy (TEM) images unveiled that the Zn-CuNCs are a large assembly of tiny nanoclusters, which become more compact in DMSO. The blue emission possesses steady-state fluorescence anisotropy, while the red emission shows no anisotropy. Further, near-perfect white light emission(WLE) was rendered with CIE coordinates of (0.33, 0.32) by combining the dual emission of the Zn-CuNCs with the original green emission of the CuNCs.



Scheme. Study of aggregation induced change in optical properties of CuNCs and its application in white light emission.

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P-150

Synthesis and characterization of liquid crystalline amide and ester bond containing benzo[1,2-g:3,4-g':5,6-g"]triquinoxaline core compounds

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New benzo[1,2-g:3,4-g':5,6-g"]triquinoxaline derivatives, BQA and BQE, with planar core are synthesized. The peripheral donor 1,2,3-tris(decyloxy)phenyl group is connected with a middle phenyl ring either through an amide or ester bond in BQA and BQE respectively. The phenyl ring is then directly connected with the core disc. The amide bond containing compound BQA exhibits liquid crystallinity with columnar hexagonal phase over wide temperature range from 230 °C down to room temperature. The ester bond containing compound BQE has an added advantage of lower isotropic temperature apart from showing room temperature liquid crystalline character. Both these compounds are thermally stable with 5% weight loss at temperature above 280 °C. They have low band gap of ~2.7eV. Columnar phases formed by the one-dimensional stacking of disc shaped molecules due to intimate π-π overlap have advantage over single crystal or amorphous polymers in terms of high charge carrier mobility, processability and ease of handling.[1][2] This enables columnar phase molecules to be utilized in organic electronic devices as an active semiconducting layer. The properties of the current compounds suggest that they can be further explored for applications in organic electronics.

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P-151

Layer-by-layer assembled Flexible Biosensor for On-Site Monitoring of *Escherichia coli*

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Escherichia coli (*E. coli*) infections primarily arise from the ingestion of contaminated food and water, posing a significant public health threat. In 2019, nearly 7.7 million people died annually by bacterial infection, with 950,000 deaths attributed solely to *E. coli,* making it the second most lethal pathogenic bacteria among the known 33 pathogens. The most lethal specie *E. coli* O157: H7 is a potent producer of shiga toxins (STEC)-stx-1, stx-2 which gets released into the bloodstream causing hemolytic anemia, thrombocytopenia, acute renal failure, and severe gut inflammation-known characteristics of HUS and HC.[1,2] Notably, no effective treatment is available; therefore, detecting it in food and water prior to consumption is the best way to mitigate the spread of infectious diseases before they escalate into pandemics.. Consequently, there is a growing need to explore more technologies for development of Point-of -Care (POC) devices to implement on-field detection. In this context, for the first time, we have designed a triple-layered smart flexible sensor (ACA) by assembling two biofilms *i.e.,* agarose (AH) and chitosan (CH) film into a sandwiched structure using the solvent casting method. This device, offers the advantages of being affordable, environmentally friendly, and highly portable, making it widely accessible to the general public, including individuals in rural or low-income communities. Also, it can be easily handled by layman and delivers fast and accurate results just by changing the color of *E. coli* contaminated samples within 30 min of the reaction with ACA**.** The material was characterized by FTIR, and SEM images gave clear visuals of each layer within the assembly. Colorimetric detection is achieved by utilizing peroxidase-mimic activity of chitosan embedded within the agarose layers, which serves as a protective barrier to preserve the catalytic activity in the long run. Through steady state kinetics, chitosan demonstrated higher affinity for H_2O_2, with a lower K_m of 0.07 mM value, compared to most of the reported literature. *E. coli* being a potent producer of β-galactosidase enzyme (as lactose metabolite), cleaves alternative β-D-(1,4) glycosidic linkages of agarose, partially exposing chitosan.[3] The oxidative degradation of chitosan by H_2O_2 produces reactive oxygen species, primarily oxidizes the chromogenic 3,3′,5,5′-tetramethylbenzidine (TMB) to yield a blue-color oxidised TMB product. The practica of ACA-thin film sensor is further established by detecting *E. coli* in various food and water samples collected from different localities of Jorhat district, Assam. Additionally, the usability and accessibility of the ACA-thin film device is enhanced by integrating it with smartphone technology. Digital images captured by smartphones can record color changes, which are analyzed by ImageJ software to extract RGB values for the quantitative determination of *E. coli.* Therefore, the ACA-thin film sensor, combined with smartphone technology, offers an innovative, user-friendly, and effective solution for the rapid detection of *E. coli* in diverse food and water samples, ultimately contributing to improved public health and safety.

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P-152

Mgo-Supported Sulfonated Graphitic Carbon Nitride: An Efficient Acid-Base Bifunctional Catalyst for One-Pot Deacetalization-Knoevenagel Cascade Reaction

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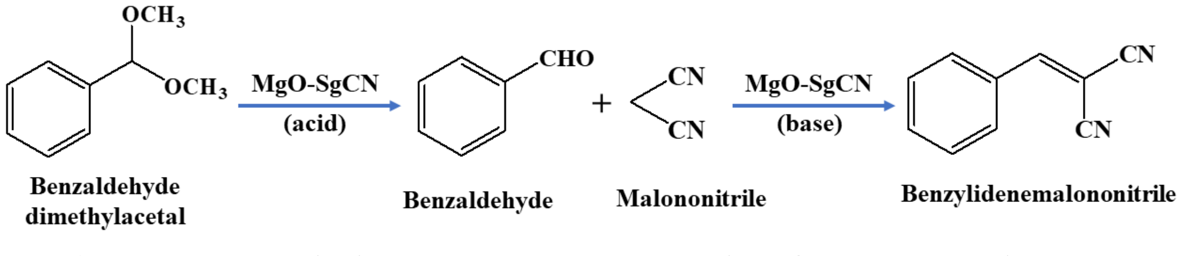
The main purpose of this work was to develop an efficient acid-base bifunctional catalyst for the synthesis of benzylidenemalononitrile through one-pot deacetalization-Knoevenagel cascade reaction. One-pot cascade reactions using heterogeneous bifunctional catalysts have garnered significant attention due to their atom-economical, time-saving, and environmentally friendly nature compared to conventional stepwise processes [1]. In this work, a novel, cost-effective, and non-toxic acid-base bifunctional catalyst was successfully synthesized by functionalizing sulfonated graphitic carbon nitride with magnesium oxide (MgO-SgCN). The sulfonation of graphitic carbon nitride (gCN) was developed by using chlorosulfonic acid to obtain sulfonated graphitic carbon nitride (SgCN) [2], followed by functionalization with magnesium oxide (MgO). The sulfonation process introduced -SO_3H groups onto the gCN surface, which conferred acidic properties to the catalyst. Given that pristine gCN has relatively weak basicity due to its conjugated structure, the incorporation of MgO was employed to enhance the basic nature of the catalyst. The physicochemical properties of the synthesized MgO-SgCN catalyst were characterized using various analytical techniques, including powder X-ray diffraction (PXRD), fourier-transform infrared spectroscopy (FT-IR), field-emission scanning electron microscopy (FESEM), field-emission transmission electron microscopy (FETEM), and nitrogen adsorption-desorption (N_2-sorption) analyses. These characterizations confirmed the successful integration of MgO into the SgCN framework. The catalytic performance of the MgO-SgCN catalyst was evaluated in the one-pot deacetalization-Knoevenagel cascade reaction between benzaldehyde dimethylacetal and malononitrile [3]. The catalyst exhibited high catalytic activity and resulted in excellent yield of benzylidenemalononitrile under solvent-free condition. Therefore, the as-synthesized MgO-SgCN catalyst provides a promising approach for efficient acid-base bifunctional catalysis in one-pot cascade reactions.



Scheme 1: One-pot deacetalization-Knoevenagel cascade reaction of benzaldehyde dimethylacetal and malononitrile.

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P-153

Thiazolidinedione- and Triazole-based Synthetic Organoselenocyanates: Potential Anticancer Activities Against Triple-Negative Breast Cancer

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Cancer has become one of the deadliest diseases worldwide, with an estimated 15 million deaths by 2040.[1] Triple-negative breast cancer (TNBC) is reported to be the most aggressive sub-type of invasive breast cancer as it lacks receptors for estrogen, progesterone hormones, and human epidermal growth factor receptor 2 (HER2).[2] Considering the limited treatment scopes and severity of TNBC, a more enhanced strategy must be developed for an effective treatment. It is evident from previous reports that heterocyclic pharmacophore-based organoselenocyanates exhibit potent anticancer activities in different organ-specific cancers.[3] In the present study, two important heterocyclic pharmacophores such as 2,4-thiazolidine-1,3-dione and 1,2,3-triazole moieties were chosen for selenocyanation to understand their selective anti-cancer activities towards TNBC cells (Figure 1).

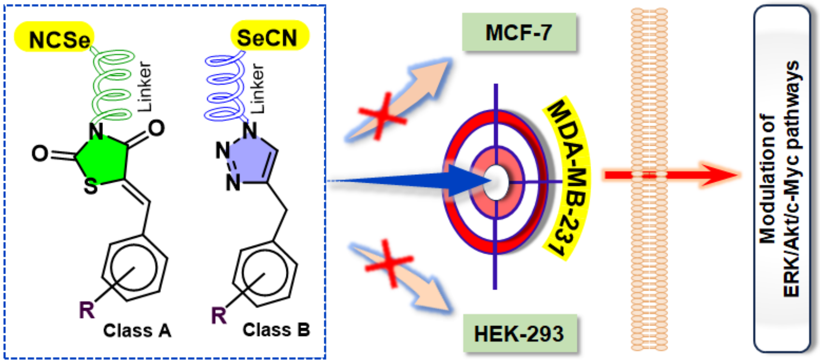

Figure 1. Schematic representation for the anti-cancer activity of novel organoselenocyanates in MDA-MB-231 cells.

Primarily a set of compounds have been designed and synthesized by incorporating selenocyanate (-SeCN) moiety to the selected heterocyclic pharmacophores. Upon the successful synthesis, their preliminary anti-cancer activities were evaluated in the representative TNBC cell line (MDA-MB-231) and in the non-malignant HEK-293 cell lines. The lead compound was selected further for the detailed investigation of its signaling pathways and mechanistic insights towards its potent anti-cancer activity. Detailed mechanistic investigations with the expression levels of key-cancer marker proteins revealed that the selected selenocyanate induced the activation of ERK pathway by upregulating *p*-ERK expression with the subsequent downregulation of *p*-Akt and c-Myc levels leading to the inhibition of cellular proliferation. Therefore, the primary outcomes of the study would be valuable towards the development of chemotherapeutic agents towards the treatment of triple-negative breast cancer.

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P-154

FLUORESCENT SCHIFF BASE SENSOR FOR SELECTIVE DETECTION OF Co(II) : APPLICATIONS IN REAL SAMPLE ANALYSIS AND CYTOTOXICITY STUDIES

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In this study, we designed and synthesized a novel and highly selective fluorescent optical sensor, N'1– ((E)-3,5-dibromo-2 hydroxybenzylidene) - N'6- ((Z)-3,5-dibromo-2-hydroxybenzylidene) adipohydrazid, via a condensation reaction in the presence of ethanol. The sensor was developed for rapid detection of Co^{2+} in an ethanol medium through a charge transfer mechanism [1]. The stoichiometry of the complexation was determined to be 1:1 using Job's plot analysis. This work highlights the development of an ESIPT (excited-state intramolecular proton transfer) active fluorescent probe, which generates fluorescence through ESIPT and a combination of fluorescence mechanisms such as aggregation-induced emission (AIE) and ESIPT [2,3]. Due to keto-enol tautomerism, the fluorophore exhibits fluorescence in both solution and solid states. The sensing mechanism was validated through experimental calculations. Importantly, the sensor demonstrated high selectivity towards Co^{2+}.

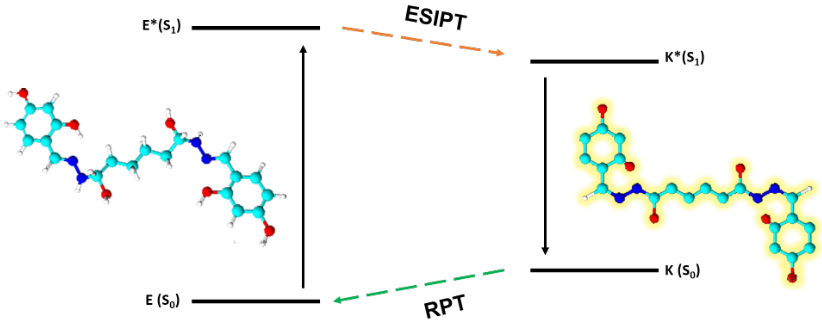

Figure 1. Graphical abstract of the ESIPT active Schiff base

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P-155

Evaluation of mode of indoleamine 2,3-dioxygenase 1 inhibition by 4,7-dichloroquinolines

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Herein, we report the development of synthetically simpler analogs of 4,7-dichloroquinoline (DCQ) as apo-indoleamine 2,3-dioxygenase 1(IDO1) protein targeting ligand to inhibit the activity of IDO1 enzyme. Derivatization of the DCQ moiety improved the IDO1 inhibitory activity both against purified enzyme and the cellular environment without any significant cytotoxicity, leading to the identification of piperazine containing DCQ derivative DCQ4 as a potent IDO1 inhibitor. A series of biophysical studies, including UV–Vis spectroscopy of the Soret band, docking, as well as protoporphyrin IX binding studies, suggested that the IDO1 inhibitory activity of potent compound could be due to its direct binding to apo-IDO1 protein and formation of DCQ4-heme complex. This simple strategy of developing apo-IDO1 targeting molecules having DCQ, piperazine, and amino acid moieties as potent IDO1 inhibitors could be useful in fighting against immune-related diseases

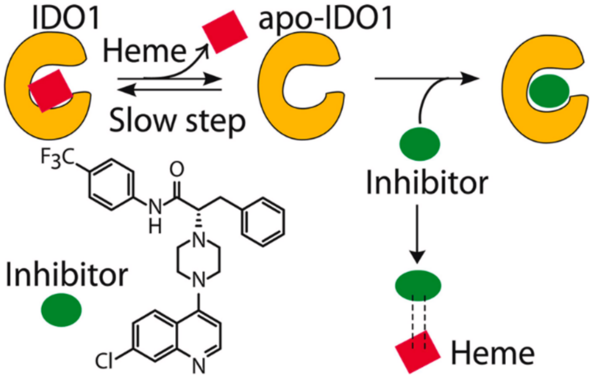

Figure 1. Graphical abstract depicting the dual mode of action for **DCQ4.**

Encouraged by the success of the apo-IDO1 inhibitor, linrodostat, in the clinical trials, we previously reported quinine derivatives that compete with heme to bind to the apo-IDO1. In continuation of our effort to develop an apo-IDO1 inhibitor, herein we report the development of 4,7-dichloroquinoline (DCQ) derivatives. The other known DCQ derivatives, such as chloroquine, hydroxychloroquine, and amodiaquine, are antimalarial drugs. The novelty of our design of compounds is the use of amino acids having a chiral center and the easy installation of piperazine moiety. The 7-chloro-4-aminoquinoline moiety of these drugs is also known to bind heme. Our comprehensive biochemical studies revealed that the potent DCQ derivative binds to apo-IDO1 and free heme to inhibit IDO1 enzyme activity.

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P-156

Aqueous Based Ultra-Small Magnetic Doped Semiconductor as a Potential Dual Imaging Probe in Biomedicine

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Substitution of semiconductor quantum dots (QDs) by a small number of transition-metal ions having magnetic properties gives rise to magnetic doped semiconductor. With the balance of optical and magnetic properties, these magnetic semiconductors are widely used in spintronics, bio-imaging and magnetic resonance imaging (MRI) applications. To facilitate their usage in bio applications, it is critical to synthesize water soluble magnetic QDs with stabilized structure while maintaining their optical and magnetic properties. Here in our work, we developed a facile substituted synthetic route to achieve Cr doped CdSe (Cr-CdSe) via a facile hydrothermal method. The effects of doping on the structural, optical, and magnetic properties of the Cr-CdSe were studied using X-ray diffraction, UV-Visible spectroscopy, photoluminescence lifetime. We then explored their chemical nature and morphology change with increase in doping concentration via X-ray photoelectron spectroscopy and transmission electron microscopy. Water soluble QDs have been used as a bio-imaging probe for the past few decades due to their strong fluorescence, photostability and improved tissue or cellular penetration. However, incorporating magnetic material into fluorescent entity harnesses the ability to control strengths of both modalities that enhance the diagnostic accuracy and facilitate its application in bio-systems especially in early accurate diagnosis. Finally, we demonstrate the competency of Cr-CdSe as a dual imaging probe with fluorescent cellular imaging and MRI applications[1–3].

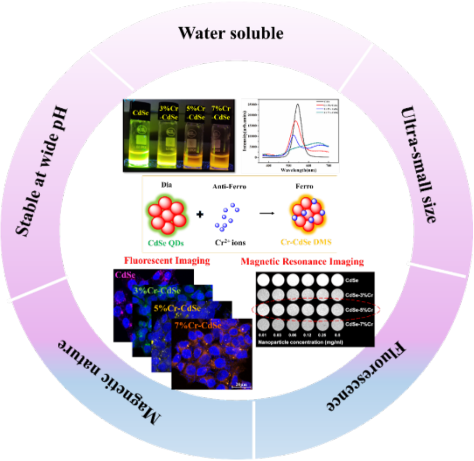

Figure 1: Graphical representation of Cr-CdSe magnetic quantum dots

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P-157

Photocatalyst Free Visible-Light-Induced Fluoroalkylative Oximation of Aryl Olefins

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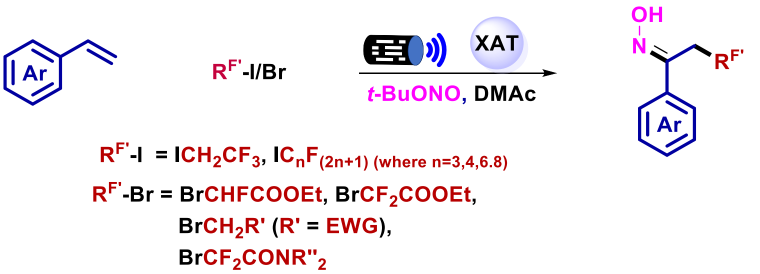
1,2-Difunctionalization of alkenes has emerged as a powerful tool for achieving novel and challenging organic transformations.[1] Recently, photocatalytic protocols without exogenous photo-redox catalysts have gained attention for their sustainability and environmental friendliness. Given the importance of fluorinated organic molecules in the domains of pharmaceuticals and agrochemcials, the direct incorporation of nitrogen and fluoroalkyl moieties provides access to novel scaffolds with brevity.[2,3]



- upto 48 examples
- commodity reagents
- broad functional group tolerance
- mild metal-free photoinduced reaction
- aryl and heteroaryl alkenes

Figure 1. Photoinduced fluoroalkyl oximation of aryl olefins using diverse class of coupling partner *via* Halogen Atom Transfer (XAT) strategy.

In this regard, we have developed a catalyst-free photochemical protocol for the fluoroalkylation-oximation of styrenyl olefins using halogen atom transfer (XAT)[4] strategy. In our stategy, three-component 1,2-difluoroalkylated oximation of the aryl olefins was accomplished under visible light irradiation. This proposed methodology provides the facile construction of new C(sp^2)-N(sp^2) bond and C(sp^3)-C(sp^3) bond in a single step transformation at the expense of C-C double bond, its applicable to multitude of substrate scope including various alkyl halides, several substituted styrenes, difluoroacetamides, and naturally-derived difluoroesters and display a broad functional group tolerance. Furthermore, the reliable scalability of the method has also been proved by the multigram scale and its practicability has also been shown by product derivatization. Control experiments offer mechanistic insights, affirming the involvement of the α-aminoalkyl radical pathway in the reaction.

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P-158

Engineering the Molecular Structure of 6-gingerol for Ceasing the Human Lysozyme Idemic Condensates

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Human lysozyme (HuL) undergoes a viscoelastic phase transition resulting in the formation of amyloid-architects that cause several pathologies including systemic amyloidosis[1]. Here we have tailored 6-gingerol by extending its molecular framework with active functional groups to specifically target HuL phase-separation events[2]. Aggregation assay revealed that engineered 6-gingerol with 4-aromatic moieties (MTV4) substantially suppressed the conversion of the lysozyme low-density liquid phase (LDLP) to solid-phase structured amyloids. The data obtained from biophysical, computational, and microscopic imaging tools suggest direct intervention of MTV4 with both liquid-like and solidified HuL condensates. Both biomolecular and computational data reveal the intrusion of MTV4 with the aggregation-prone hydrophobic stretches within the HuL, thereby retaining the native macro-state and reversing the misfolded conformers to highly dynamic monomers. These residues fall under the β-sheet-containing sub-domain B, which is found to be a crucial part of the irreversible fibril core[3]. Also, MTV4 was able to induce rapid fragmentation of preformed-toxic amyloid fibrils. These results reinforce the importance of the short-range hydrophobic interactions involving Π-electrons in preventing human lysozyme liquid−liquid phase separation (LLPS).

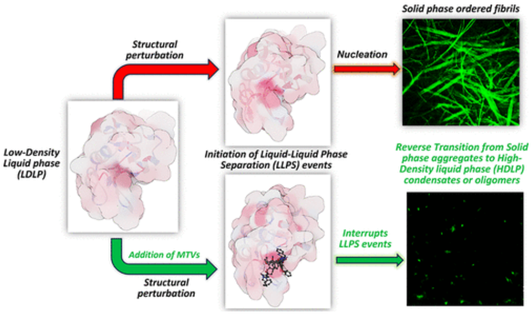

Figure 1. Schematic overview of Human lysozyme undergoing aberrant LLPS and the effect of MTV4 on mitigating such transition under in vitro conditions

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The Hidden Chemistry of Weeds: Unveling Phytochemicals for Nutritional and Therapeutic Benefits

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The increasing demand for nutritious, high-quality food has boosted interest in functional foods and natural remedies, prompting the search of alternative food sources with health benefits. Weeds, often seen as undesirable plants, compete with crops for light, water, and nutrients, leading to their bad reputation in agriculture. Known for their violent growth and unsightly appearance, weeds are generally regarded as nuisances that hamper the plant growth and decrease crop yields[1, 2]. However, this perception oversees the fact that many weeds hold valuable nutritional and medicinal properties due to their rich phytochemical content[3].

Phytochemicals such as alkaloids, flavonoids, tannins, terpenoids, and saponins are accountable for many of the therapeutic benefits of weeds, making them brilliant candidates for use in herbal medicine and natural remedies[4]. For example, **Purslane** (*Portulaca oleracea*) is known for its high content of flavonoids, fatty acids, and alkaloids, it offers strong anti-inflammatory and antioxidant benefits. Purslane is not only consumed as a nutrient-rich wild vegetable but is also used in traditional medicine to reduce inflammation and protect heart health[5]. Despite efforts to harness these properties, many weeds remain underexplored, representing unexploited resources that could improve food security, offer nutritional benefits, and create new economic opportunities for rural communities. By raising awareness of their medicinal and practical value, this study aims to shift the perspective on weeds, highlighting their potential as valuable resources that grow naturally, without added cost or effort from farmers.

Hence, to accomplish this, the present review article is intended to compile the research on the nutritional and phytochemical composition of several weed species, explore their diverse applications and health-promoting potential.

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P-160

Photocatalytic CO_2 Reduction to Methanol Integrated with the Oxidative Coupling of Thiols to S-X (X=S, C) bond formation over $Fe_3O_4/BiVO_4$ Composite

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A dual functional approach for CO2 reduction coupled with oxidative organic synthesis in a single reaction system is a promising way to get CO2 reduction products with the coproduction of high-value chemicals using light energy under mild conditions. Herein, we report an integrated approach in which CO2 acts as an oxidant that affords the oxidative homocoupling of thiols to disulfides and cross-coupling with organohalides to thioethers along with the simultaneous production of methanol over a heterostructured composite of iron (III) oxide and bismuth vanadate (Fe3O4/BiVO4) under visible light irradiation. The developed protocol provides an economical and fascinating organic synthesis combined with methanol production by simultaneously utilizing photo-excited electrons and holes more efficiently in a single reaction system. Hence, the present study opens up new opportunities for solar fuel generation from CO2 integrated with the synthesis of value-added fine chemicals.

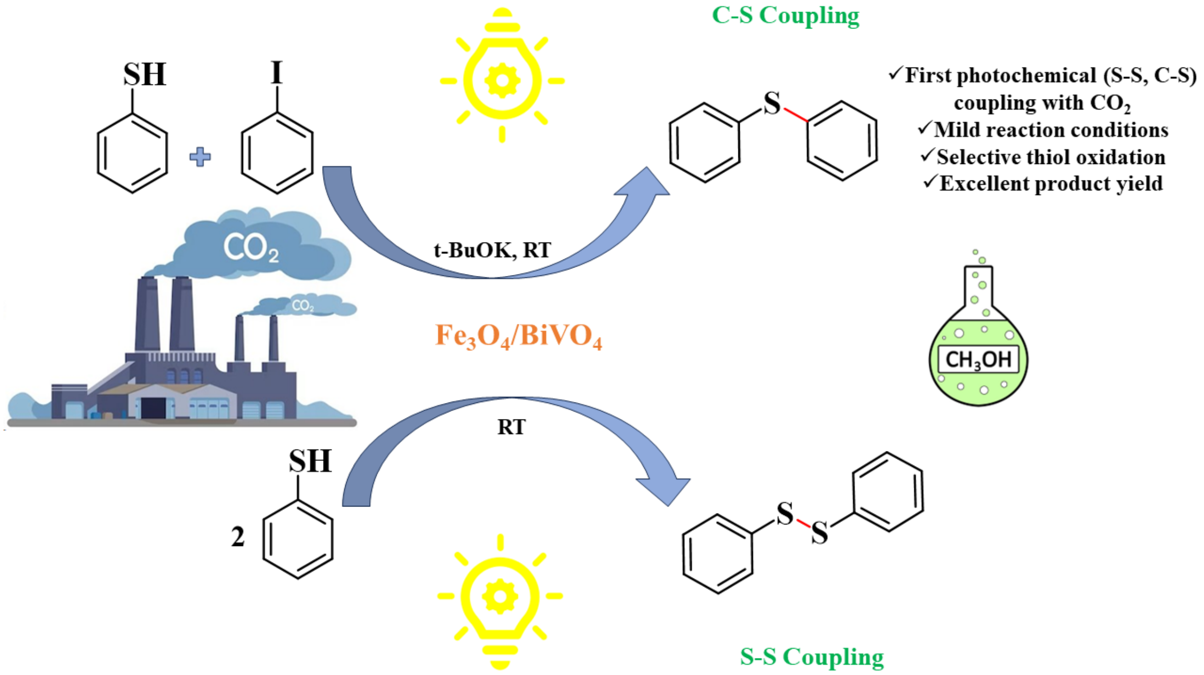

Figure 1. Graphical abstract on Oxidative Coupling of Thiols to S-X (X=S, C) bond formation

P-161

Hollow Cuboidal Metal Oxide-Based Asymmetric Electrode Configuration for High-Performance Anion Exchange through Quaternized Pyridine-Poly(vinyl alcohol) @ Metal Hydroxide Nanosheets for Water Dissociation

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Functionalization plays a pivotal role in enabling the deliberate design of membranes to be tailored as an anion exchange or a cation exchange, thereby yielding improved ion exchange capacity. In this study, we have engineered a bipolar membrane (BPM) by integrating quaternized pyridine-functionalized poly(vinyl alcohol) (PVA) as an anion exchange membrane (AEM), combined with an activated Nafion as the cation exchange membrane (CEM). The ion exchange capacity (IEC) measurements revealed that the synthesized AEM possesses an IEC value of 2.3 mmol/g, a measure equivalent to the values characteristic of the most effective commercially available AEMs. The hybrid BPM fabricated through the incorporation of β-$Ni(OH)_2$ nanosheets between the AEM and CEM was found to be remarkably enhancing the water dissociation (WD) reaction and exhibiting a substantial 55.7% increase in water uptake capacity. Incorporating a unique asymmetric electrode setup having hollow cuboidal CuO significantly boosted the efficiency, enhancing overall water-splitting and dissociation facilitated by the BPM. Systematic experimentation revealed our system's proficiency, achieving a remarkable 0.90 V at $\Delta pH \approx 0$ with a current density of 5.52 mA/cm^2, and 0.91 V at $\Delta pH \approx 12$ providing 7.40 mA/cm^2, showcasing reduced voltage requirements for the water dissociation process.

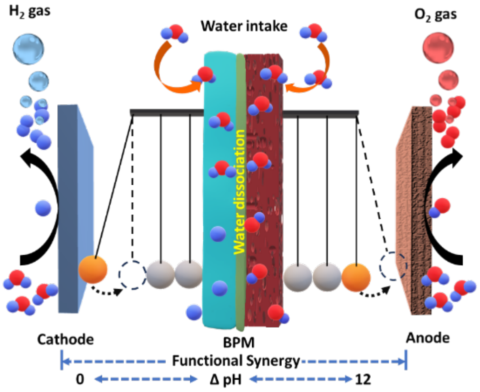

Figure 1. Synergistic interplay between a bipolar membrane (BPM) and an asymmetric electrode arrangement within an H-cell configuration facilitates an efficient overall water dissociation

The study demonstrates the fabrication of a high-performance bipolar membrane (BPM) using pyridine-functionalized PVA as the anion exchange membrane (AEM) and activated Nafion as the cation exchange membrane (CEM), with β-$Ni(OH)_2$ serving as the water dissociation catalyst (WDC) in the interlayer. Functionalizing PVA with pyridine improved water uptake by increasing hydrophilicity and rendered the polymer water-insoluble via an acetalization reaction with 2-pyridinecarbaldehyde. The incorporation of β-$Ni(OH)_2$ enhanced water dissociation efficiency, reducing the required transmembrane voltage from 1.05 to 0.90 V at $\Delta pH \approx 0$ and from 1.20 to 0.91 V at $\Delta pH \approx 12$. Additionally, an asymmetric electrode system using Pt for hydrogen evolution and hollow cuboidal CuO on nickel foam for oxygen evolution further improved current density and water dissociation efficiency. A 25-hour stability test at 25 mA/cm^2 showed negligible changes in voltage, confirming the stability of the BPM.

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P-162

INTERACTION OF METAL IONS WITH TWO SCHIFF BASES OF SALICYLALDEHYDE

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ABSTRACT

Condensation of Salicylaldehyde with p-Toluidine and with 1-Napthalamine [1,2] were performed to give two Schiff bases (S1 & S2), and their structures have been confirmed by using different spectroscopic methods i.e., UV-Visible, IR and other spectroscopic techniques. The binding interactions of the ligands with a series of transition metal ions such as Cu (II), Zn (II), Ni (II) and Co (II) were studied, as metal complexes of Schiff bases have wide applications in different areas [3,4]. The possible biological activities of the metal complexes of the two Schiff bases prepared are under investigation.

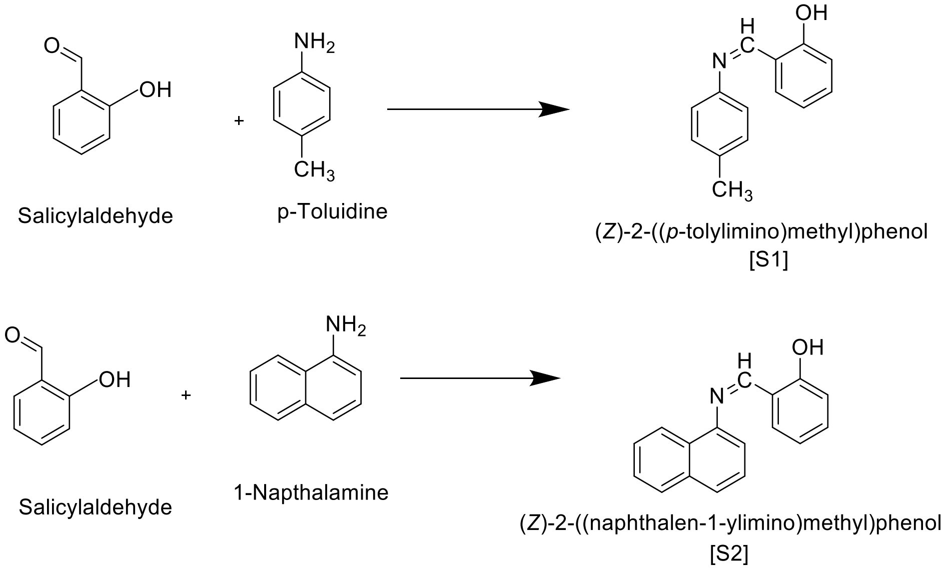

Fig1: Synthesis of Schiff bases (S1&S2)

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P-163

Micelle-assisted ultrafast sensing of cyanide via twisted-intramolecular-charge-transfer based fluorogenic nano-probes

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Amongst various anions, cyanide (CN^-) is considered one of the most poisonous anions on account of its extreme toxicity towards human. Even at a very low concentration it causes serious health issues such as histotoxic anoxia, eventually leading to death. Despite such hazardous nature of CN^-, it still finds widespread use in various industries such as metal mining, jewellery manufacturing, electroplating, *etc.* Therefore, there is growing interest in the development of highly selective as well as sensitive artificial chemosensors for CN^-, especially in aqueous medium. The most commonly employed approaches for CN^- detection encompass the hydrogen bonding approach, chemodosimetric method, and deprotonation reaction-based sensing. However, the high solvation energy of CN^- makes it very difficult to achieve its effective or efficient sensing in aqueous medium. So, there is still much room for improvement in terms of achieving superior sensitivity, selectivity, and applicability. In this presentation, we are going to review our recent work on CN^- sensing where we have shown for the first time that utilizing a TICT (twisted intramolecular charge transfer) active probe in the micellar medium could help in developing highly sensitive, and selective cyanide sensors and a systematic study on substituent dependency of such a sensing process with the assistance of a micellar system.

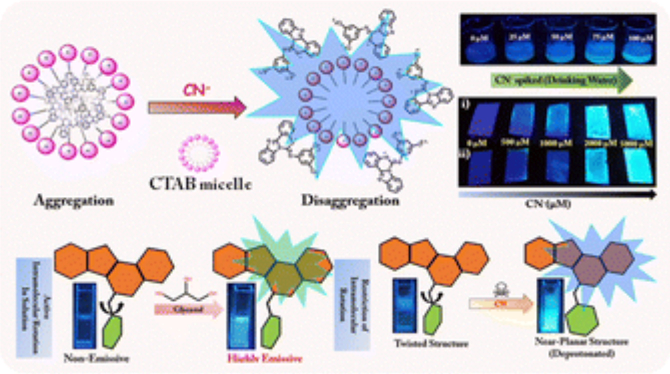

Figure 1. Graphical abstract of the micelle-assisted CN^- sensing *via* TICT active probe.

Twisted benzimidazoquinazoline based fluorogenic probes (Benz-d-CF_3 and Benz-m-CF_3) with varying pi-acidic terminal substituents showed TICT (twisted intramolecular charge transfer) behaviour. They formed self-assembled nano-aggregates in an aqueous CTAB medium, and only Benz-d-CF_3 displayed a selective fluorescence turn-on response toward CN^- in a 100% aqueous medium. However, the sensitivity and selectivity of fluorescence sensing towards CN^- enhanced exponentially in aqueous medium in the presence of CTAB. Probe Benz-d-CF_3 had a detection limit as low as 496.5 nM and a high-speed fluorescence response time, which promises its practical application for detecting CN^- in drinking water. The assistance of micelle systems facilitates a very fast, sensitive and selective detection of CN^- in water. The sensitivity as well as selectivity of the probes towards CN^- can just be fine-tuned by varying their terminal substituents.

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P-164

Conformation-dependent excited state properties in extended π-conjugated systems

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Understanding the intricate relationship between the different possible conformers and the photophysical/excited-state properties plays a crucial role in the design of efficient electronic devices. In this aspect, we will present how the excited state properties vary in different conformers of ***cis-*** and ***trans-*** 2,2’-Bipyridine oligomers ((BPY)n). For this, we constructed ***ortho-(o-), meta-(m-),*** and ***para- (p-)*** conformers of ***cis-*** and ***trans-*** 2,2’-(BPY)n. At n=4, the ***trans-o-*** and ***m-*** isomers formed a linear structure where ***o-*** has a planar backbone, whereas the ***p-*** isomer has a non-linear and non-planar structure, shown in Figure 1. Excited state characterization reveals that the S_1 state of ***o-*** and ***m-*** has a partial charge transfer character, whereas for ***p-*** isomer, the S_1 is a purely local state.

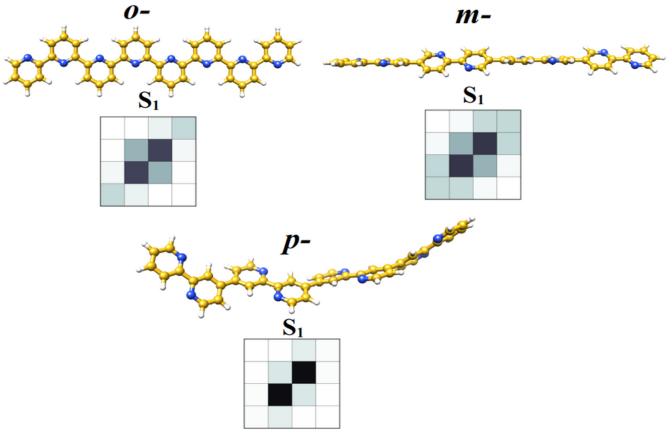

Figure 1. Ground state geometries of ***ortho-***, ***meta-***, and ***para-*** isomers of ***trans***- 2,2’-(BPY)$_4$ and their S1 state electron-hole correlation plots.

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P-165

A Lewis Acid-Catalyzed Cascade Synthesis of Fused *N*-Heterocycles from 2-Alkynylanilines and 2-Formylbenzonitriles: Unveiling Iminoisoindoloindolone and Its Derivatives

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We herein reveal a streamlined synthesis of structurally fused 6-iminoisoindoloindolones via a meticulously orchestrated cascade reaction. This process seamlessly intertwines 2-alkynylaniline and 2-formylbenzonitrile under the catalytic influence of TMSOTf, giving rise to these compounds in remarkable yields that stand as a testament to the efficiency of our approach. Moreover, the versatility of this synthetic strategy extends far beyond mere synthesis, offering a gateway to the creation of both isoindoloindolone and unprecedented diphenylbenzopyrrolizinoisoquinolinone derivatives, thereby opening new horizons in the realm of chemical innovation. Furthermore, the strategic elegance of this synthetic methodology is underscored by its potential for scale-up production and applicability across diverse chemical contexts.

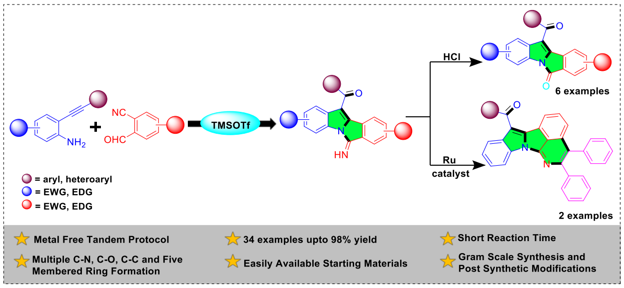

Figure 1. Graphical abstract of the synthesis of iminoisoindoloindolone and its derivatives

Multifused *N*-heterocyclic compounds represent some of the most versatile and significant heterocyclic scaffolds, abundant in natural products with diverse medicinal importance and widespread natural occurrence. Their pivotal roles in the pharmaceutical industry and material science have garnered considerable attention in recent years. Among the plethora of fused *N*-heterocyclic motifs, indole-fused polycyclic scaffolds stand out for their prevalence in numerous heterocyclic compounds, exhibiting remarkable physiological and biological activities across natural products, medicines, and agrochemicals. The past few years have witnessed a surge in interest toward synthesizing indole derivatives, driven by the potential to design polycyclic structures incorporating multiple fused heterocyclic scaffolds, thus offering avenues for creating novel heterocycles with both chemical and biomedical implications. We present herein a simple and concise strategy yielding fused 6-imino-6*H*-isoindolo[2,1-*a*]indolone and its derivatives from 2-alkynylaniline and 2-formylbenzonitrile in excellent yields. The reaction progresses in a cascade fashion under the catalytic action of TMSOTf.

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Bimetallic MOF Templated Nanocomposites of Molybdenum Oxide for Water-Splitting

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As the demand for sustainable and renewable energy solutions increases, electrocatalytic water splitting has emerged as a key process for producing clean hydrogen fuel. Metal-Organic Frameworks (MOFs), with their tunable structures, high surface area, and ability to host diverse catalytic sites, have garnered significant attention for their potential to improve water-splitting efficiency[1]. However, designing MOF-based systems with enhanced electrocatalytic properties remains a challenge. In this study, we explore the use of bimetallic MOF-supported catalysts for water splitting, demonstrating their superior performance compared to traditional systems.

A series of bimetallic Zeolitic Imidazolate Frameworks (ZIFs) were synthesized by varying the proportions of cobalt (Co) and zinc (Zn) to form a robust bimetallic template. These templates were further functionalized with molybdenum oxide (MoO_x) nanoparticles[2], which are known for their excellent catalytic activity in water-splitting reactions. The resulting composite material was characterized using a suite of analytical techniques, including Powder X-ray Diffraction (PXRD), Scanning Electron Microscopy (SEM), Energy Dispersive X-ray (EDX) analysis, Infrared Spectroscopy (IR), Brunauer–Emmett–Teller (BET) surface area analysis, and Thermogravimetric Analysis (TGA), to thoroughly investigate the structural, morphological, and thermal properties.

Electrochemical studies revealed the promising electrocatalytic performance of the MoO_x-deposited bimetallic ZIFs in both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), demonstrating remarkable stability and efficiency[3]. Additionally, computational simulations were performed to gain a deeper understanding of the catalytic mechanism and the role of the MOF-supported system in enhancing water splitting. These insights offer valuable perspectives on the structure-property relationships that govern catalytic activity in MOF-based systems.

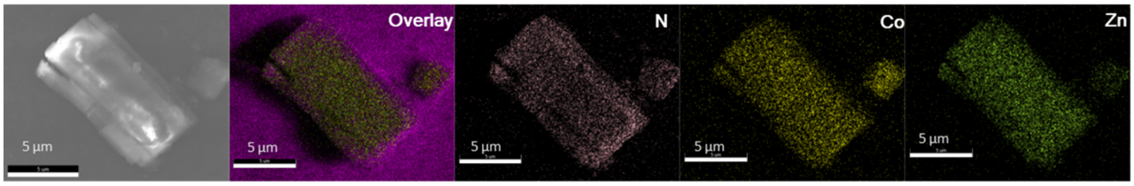

Figure 1. SEM of Co-Zn mixed metal ZIF

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Synthetic Benzylic Diselenides and Disulfides: Potential Anticancer Activities via Modulation of the ROS-Dependent Akt/β-Catenin Signaling Pathway

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The natural and synthetic organoselenium compounds have garnered much research attention due to their chemotherapeutic and chemopreventive activities against different organ-specific malignancies.[1] With the global growth in breast cancer incidences, our research is focused on the development of new strategic treatment approaches for triple-negative breast cancer (TNBC) due to its aggressive nature and lack of targeted therapies [2]. In this work, we describe the synthesis of a series of benzylic diselenides (**1-6**) and disulfides (**7-12**), and their mechanism of anticancer activities in triple-negative breast cancer cells (MDA-MB-231) [3].

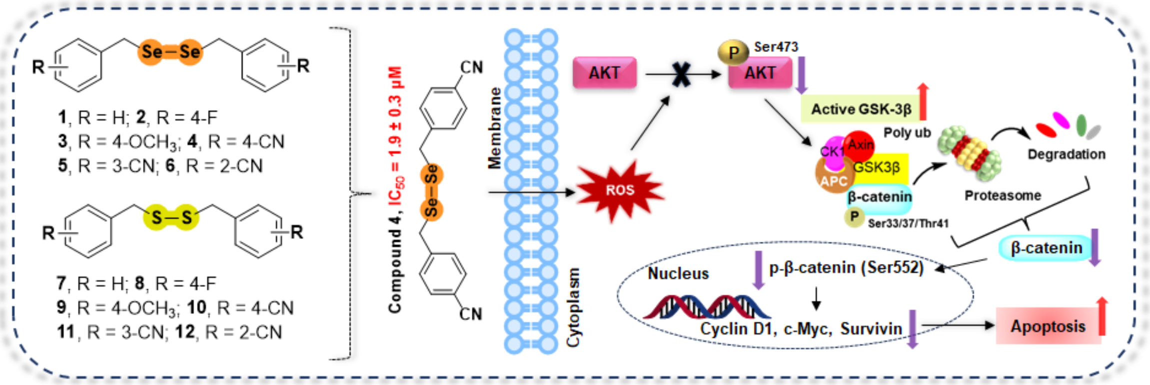

Figure 1. Graphical abstract depicting the chemical structures of the benzylic diselenides (**1-6**) and their corresponding disulfides (**7-12**); and the plausible mechanistic insight into the anticancer activities of diselenide **4**.

Preliminary anti-proliferative activities indicated 4-cyano-substituted diselenide **4** to be most potent with an IC_{50} value of 1.9 ± 0.3μM. Detailed mechanistic investigations showed that diselenide **4** induces apoptosis and causes G1 phase arrest of the cell cycle. It exhibits anticancer activity by suppressing the Akt/β-catenin signaling pathway. Further control experiments with LiCl (inhibitor of GSK-3β) revealed that down-regulation of β-catenin was promoted by GSK-3β-induced phosphorylation of β-catenin and its subsequent proteasomal degradation. Moreover, the intracellular ROS was found to act as an upstream mediator for the inactivation of the Akt/β-catenin signaling pathway. The present study describing the efficient anticancer activity of a synthetic benzylic diselenide towards triple-negative breast cancer cells through the modulation of ROS-dependent Akt/β-catenin signaling pathway would certainly be helpful in the future towards the development of small-molecule organoselenium compounds for the treatment of cancer.

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P-168

Two Sustainable Pathways of MOF-Catalysed Room Temperature Chemical Fixation of CO_2 Inside Alkynes Under Atmospheric Pressure

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ABSTRACT

The remarkable uphill of the environmental CO_2 concentration during the past few decades through numerous bio-activities demands the development of effective materials to mitigate CO_2 concentration in the air. Utilization of adsorbent materials for the reversible physisorption of CO_2 has significantly less impact. Hence, the development of functional solid-state materials for efficient capture and irreversible chemical conversion of CO_2 into valuable fine chemicals is highly demanding. Recognizing this need, herein, we demonstrate the construction and characterization of a nitrogen-rich, aqua-stable, Ag(0)-nanoparticles doped metal-organic framework (MOF) and its catalytic application for the chemical fixation of CO_2 in an irreversible manner. In the present study, we showcase two sustainable pathways of CO_2 fixation for the preparation of important commodity chemicals. The designed catalyst (MOF@Ag NPs), displayed excellent catalytic activity for the cyclization of various propargylic amines and propargylic alcohols with CO_2 under atmospheric temperature and pressure conditions. Notably, MOF@Ag NPs is capable of facilitating both of these conversions at room temperature and atmospheric pressure of CO_2. This is the first MOF-based catalyst effective for the quantitative chemical conversion of propargylic amine at room temperature and under atmospheric pressure of CO_2. With this catalyst, we successfully transformed CO_2 (a major greenhouse gas) into 2-oxazolidinones and α-alkylidene cyclic carbonates, which are largely found in various agrochemicals and pharmaceuticals. Furthermore, our catalyst exhibited high recyclability, retaining its catalytic activity and structural integrity over several cycles of reuse. Several control experiments indicated that the remarkable catalytic activity of MOF@Ag NPs was due to the presence of highly exposed alkynophilic Ag(0) catalytic sites distributed on the pore walls of MOF. This work showcases the promising application of MOF@Ag NPs in maintaining environmental sustainability and converting CO_2 into valuable bio-active commodity chemicals under ambient conditions.

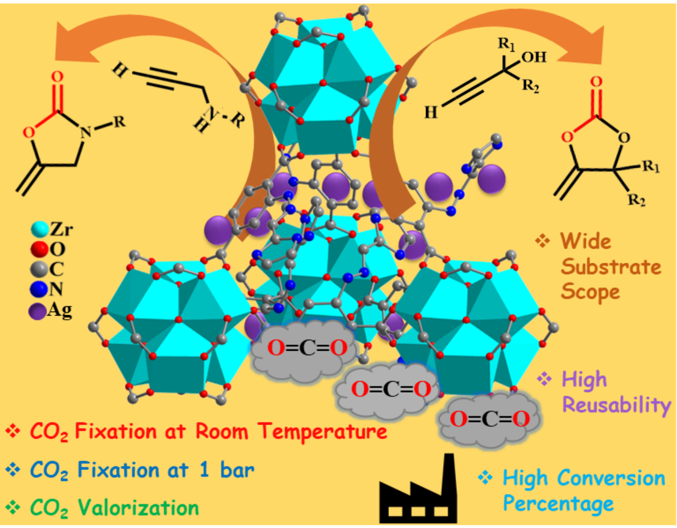

Figure 1. Graphical representation of our newly developed MOF@Ag NPs system towards CO_2 fixation.

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Detailed Studies on the Photoluminescence Properties of Wet Chemically Grown Eu-doped Wrinkled ZnO Nanorods

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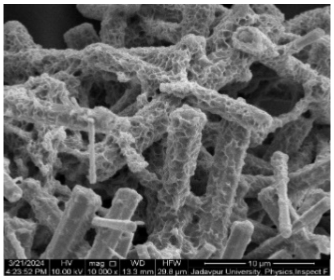
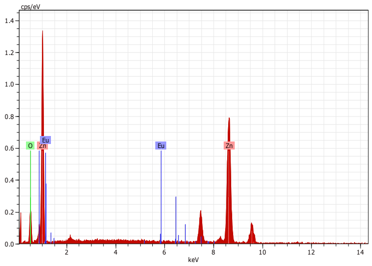
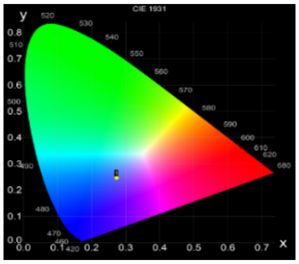
In recent years, Photoluminescence (PL) has emerged as a vital tool for developing advanced optoelectronic devices, especially in applications such as LED's, displays and bio-imaging. The ability to tune the optical properties of materials like Zinc Oxide (ZnO) through doping has gained significant attention. This study presents the growth of europium (Eu)- doped ZnO nanorods via a wet chemical process, on nickel (Ni) foam. The X-ray diffraction (XRD) confirmed the crystalline nature of ZnO, with no secondary phases from Eu doping. Field emission scanning electron microscopy (FESEM) revealed a rod-like morphology in pure ZnO, while Eu-doped ZnO exhibited surface wrinkles on the rods, suggesting a modification in growth behaviour due to the Eu incorporation. Energy-dispersive X-ray spectroscopy (EDX) analysis shows the presence of Eu in the ZnO matrix.

The PL studies demonstrated emission properties from Eu-Doped ZnO, providing insights into the electron-hole recombination dynamics influenced by the Eu ions. The results suggest that Eu doping significantly alters the optical characteristics of ZnO, making it a promising candidate for optoelectronic applications. The structural modification and enhanced PL are discussed in relation to the material's potential for use in light emitting devices.







Keywords: ZnO, Europium, Photoluminescence, optoelectronic devices.

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P-170

Iodine Promoted *N*-acylation of sulfoximines *via* Oxidative C=C Bond Cleavage of Cinnamic Acids

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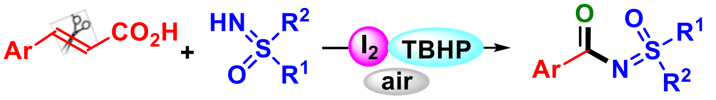
An iodine-promoted C□C bond cleavage [1] with concomitant decarboxylation and cross-coupling between cinnamic acids and *NH*-sulfoximines has been developed. This reaction proceeds *via* selective C=C bond cleavage, followed by decarboxylation and oxidative sulfoximidation. [2,3] This metal- and base-free protocol involves dioxygen as the source of oxygen, which is facilitated by *tert*-butyl hydroperoxide (TBHP) as the oxidant. This leads to aldehydes as intermediates, which then undergo coupling with sulfoximine to yield the desired product. This chemistry offers a new and alternative way for the synthesis of a wide range of *N*-acyl sulfoximines products [4,5] which is a useful synthetic intermediate in organic synthesis and a vital skeleton for natural products.



- ***C=C bond cleavage***
- ***Decarboxylation***
- ***C=O, C N bond formation***
- ***Metal- and base-free strategy***
- ***35 examples, upto 81% yield***
- ***One-pot, mild reacton conditions***

Figure 1. Graphical representation of sulfoximidation of cinnamic acids

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P-171

Fabrication of robust and versatile ionic thermoelectric devices of natural clay minerals

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Due to advantages like high Seebeck coefficients, simple fabrication techniques, and use of abundant elements, ionic thermoelectric (i-TE) devices are emerging to be an ideal tool for harvesting low-grade waste heat. However, high dependence on humidity and poor thermal stability of organic polymers/polyelectrolytes/ionic liquids are restricting the utility area of i-TE devices. To expand the horizon of applicability, here, thermally and chemically robust natural clay minerals are explored for fabricating i-TE devices. Devices prepared with exfoliated layers of clay showed high Seebeck coefficients (6 ± 0.8 mV/K), which is significantly improved (up to 140 %) upon functionalization with the –SO_3H groups (14.4 ± 0.4 mV/K). i-TE devices of clay exhibit unique advantages like thermal robustness and water-induced damage healing ability. These devices did not show any sign of deterioration even after exposure to 300 °C. Along with waste heat, clay-i-TE devices can also convert abundant sunlight energy into electricity. Upon being coated with polyvinyl alcohol (PVA), borax, and LiCl-based hydrogel the performance of the i-TE device at low-humidity conditions is drastically improved. The possibility of practical utility of clay-based i-TE devices was demonstrated in areas like fire alarms, touch sensors and electricity generation from hot water steam.

P-172

Potential-dependent Oxygen Evolution Reactions on Fe-NC Materials

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Electrochemical water oxidation reactions play a major role in the context of sustainable energy storage, productions. However, thermodynamic bottleneck of overpotential for oxygen evolution reactions restricts the materials for full-scale applications. While, tremendous experimental research has been done for better electrocatalyst design for OER over last couple of years, a thorough understanding about the catalysts in the operando conditions is lacking. Keeping focused in this direction, we are taking single Fe atom doped graphene i.e. well known Fe-NC materials as a model systems to build a electrochemical model from the first-principle calculations to decifer the role of the electrochemical potential, metal electronic structures. In our studies, we have observed that our developed grand-canonical based quantum mechanical calculations nicely captures the real electrochemical mechanisms over the Fe-NC materials.

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P-173

First Asymmetric Total Syntheses of Avapyran and Dysiquinol D

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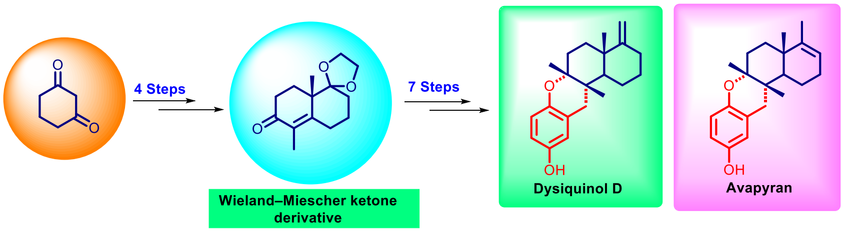
Avapyran was isolated from the Okinawan marine sponge *Dysidea sponge* by Yamazaki and his coworkers in 2016.[1] Dysiquinol D was isolated from the South China Sea marine sponge *Dysidea avara* by Lin and coworkers in 2015.[2] In Avapyran and Dysiquinol D, a chromane moiety is connected to a *trans*-avarane moiety, forming a 6-6-6-6 tetracyclic system. From the preliminary investigation of biological activity, it is found that Avapyran shows inhibitory activities against protein tyrosine phosphatase 1B (PTP1B) with IC_{50} value 11 µM and Dysiquinol D showed cytotoxicity and NF-kB inhibitory activities with IC_{50} values of 2.8 and 0.81 mM. Till now, no studies on the syntheses of these bioactive sesquiterpenes have been reported. We have developed a convergent route to these sesquiterpenes from 1,3-Cyclohexadiene over 11 steps.[3] Stereoselective reductive benzylation followed by intramolecular cyclization reactions were used for the installation of *cis*-benzo chromane moiety.



Scheme 1. Total syntheses of Avapyran and Dysiquinol D.

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P-174

Tuning Proton Conductivity in MOF-GO Composites by Modulating Graphene Oxide Content

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Metal-organic frameworks (MOFs) have emerged as crucial materials for proton conductivity, especially in the context of the growing need for alternative energy sources. Enhancing the proton conductivity of MOFs has been a major focus, with one effective approach involving the integration of MOFs with graphene oxide (GO) to form composite materials. In this study, Cr-MIL-101 has been selected, and its growth on GO sheets is achieved through *in-situ* crystallization, leading to the formation of MOF-GO composites with varying GO contents, (**MIL-101/GO(*x*%)**, $x = 1\%$, 2%, and 5%). The oxygen functional groups on the 2D-GO layer, like carboxyl, hydroxyl, and epoxy groups, improve both the acidity and hydrophilicity of the composite, which directly contributes to improved proton conductivity. All the composites exhibit higher conductivity than that shown by the parent MOF due to the additional acidic functional groups introduced by GO. Among the different composites, the **MIL-101/GO(2%)** composite exhibits the highest proton conductivity, achieving 0.105 S cm^{-1} at 80 °C and 98% relative humidity (RH). These results highlight the potential of MOF-GO composites for application in proton exchange membranes and other energy-related technologies.

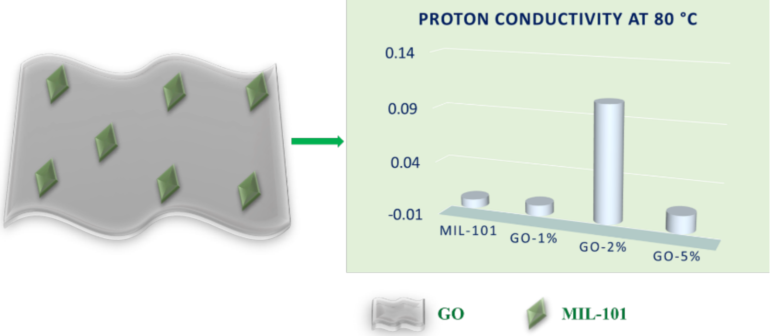

Figure 1. Graphical abstract Showing proton conductivity of MIL-101-GO composites with different GO content.

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P-175

Selective N-Arylation of Thiopurine using C-F Bond Activation of Fluorobenzene: Emerging Drug against Prostate Cancer

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The carbon-fluorine (C-F) bond, known for its exceptional strength, presents a significant challenge for activation in organic synthesis.[1] The present introduces a novel heterogeneous[2], ligand-free method to overcome this difficulty by selectively synthesizing N-arylated thiopurine conjugates through the activation of C-F bonds in fluorobenzene. The catalyst used in this process is copper oxide nanoparticles (CuO-NPs) immobilized with an ionic liquid, which facilitates the efficient activation of C-F bonds. This innovative approach enables the precise synthesis of a wide range of thiopurine conjugates with remarkable functional group tolerance. The method produces impressive product yields, nearing 90%, showcasing its efficiency. The successful activation of C-F bonds underscores the potential of this methodology for developing thiopurine conjugates, compounds with promising medicinal applications. To verify the effectiveness of the synthesized nanocatalyst, several advanced characterization techniques were employed, including field emission scanning electron microscopy (FE-SEM), Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), energy-dispersive X-ray spectroscopy (EDS) with mapping images, Brunauer–Emmett–Teller (BET) surface area analysis, and powder X-ray diffraction (P-XRD). These analyses confirm the nanocatalyst's efficiency and its potential for broader use in advanced chemical synthesis.

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P-176

Alcohol Dehydrogenases and their Potential Applications

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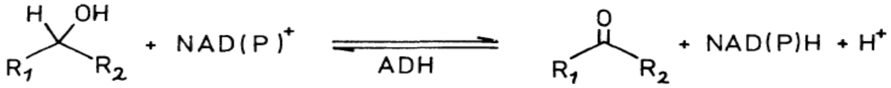
Alcohol dehydrogenases are highly diverse type of holoenzymes that occurs in many plants, animals and in micro-organisms and facilitates the inter-conversion between carbonyl compounds and corresponding alcohols (primary and secondary) using reduced and oxidized form of nicotinamide adenine dinucleotide i.e., NADH and NAD^+ as co-factors for electron donation and acceptance.[1]



Alcohol dehydrogenases may be broadly classified into three major families; medium chain dehydrogenases/reductases (MDR family, ~370 residues, zinc containing), short chain dehydrogenases/reductases (SDR family, ~250 residues, lacks metal ions) and iron containing/activated alcohol dehydrogenases. The activity of first category of the enzymes is predominantly observe in higher animals, plants and in yeast whereas the second category mainly observed in insects and the third category of dehydrogenases were isolated from thermophiles and hyperthermophiles. [2][3][4]

One of the most important applications of ADHs includes production of chiral pharmaceutical intermediates. Based on their high stereoselectivity under mild conditions, they have been used in asymmetric synthesis of chiral alcohols which acts as intermediate to produce antidepressants, antianxiety, antiasthmatics, anticholesterol, antihypertensive, antithrombotic, antiepileptic, anti-inflammatory, anticancer, antiemetic, β-Lactam antibiotics and many more drugs.[5][6]

Other important application involve selective reduction of α,β-unsaturated carbonyl compounds to their corresponding unsaturated alcohols, a very important chemical conversion for flavor and fragrance industries. Selective reduction of cinnamaldehyde to cinnamyl alcohol by conventional method is very difficult to achieve. α,β-unsaturated carbonyl compounds and other carbonyl compounds are reversibly reduced to corresponding alcohols in presence of alcohol dehydrogenase enzymes. The reactions in presence of ADHs are very much efficient with high yield and is free from any side products.[7]

Other important application includes the synthesis of fine chemicals of industrial importance like γ-Valerolactone, optically active phenylethanols, and butanediol.

Keywords: Alcohol dehydrogenase - NAD^+ / NADH – pharmaceuticals- flavor and fragrance.

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P-177

Dichalcogen, Halogen and Charge Assisted Hydrogen bonded Assemblies in Pyrazole-based Coordination Compounds of Ni(II), Mn(II) and Cu(II): Anticancer Activities and Theoretical Studies

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Researchers are interested in the intriguing network architecture and applications of coordination solids, which involves the self-assembly processes of molecular building blocks directed by conventional and novel supramolecular interactions [1]. Although non-covalent interactions such as hydrogen bonding, π-π stacking, anion-π, cation-π, σ/ π hole, halogen bonding interactions are referred as weak but their cumulative effect plays a crucial role in the overall stability of the supramolecular architecture [2,3]. Unconventional Cl···Cl contacts have also received significant attention in supramolecular chemistry, which can also be considered as donor–acceptor interactions [4,5]. Because of their significance in supramolecular assemblies, molecular biology, and crystal engineering, non-covalent interactions have been the subject of interest for investigators [3]. In order to assemble structures with the necessary dimensionalities, it is also important to select the appropriate metal centers and organic moieties in combination with favorable reaction conditions [6,7]. Pyrazole and its derivatives have been extensively employed to design coordination compounds owing to their various pharmacological activities, *viz*. anti-inflammatory, analgesic, anticancer, antimicrobial etc. and hold a unique place from the medicinal chemistry viewpoint [1].

Herein, we have synthesised and characterized three coordination complexes of Ni(II), Mn(II) and Cu(II) [Ni(H_2O)$_4$(Hdmpz)$_2$]ADS (**1**); [Mn(H_2O)$_4$(Hdmpz)$_2$]ADS (**2**) and [Cu_2(□-Cl_2)Cl_2(Hdmpz)$_4$] (**3**), where Hdmpz = 3,5-dimethylpyrazole; ADS = anthraquinone-1,5- disulfonate). Crystal structure analysis of the compounds **1** and **2** reveal the presence of unconventional O···O dichalcogen bonding interactions along with aromatic π-stacking, charge assisted O–H···O and C–H···O hydrogen bonds. However, crystal structure analysis of compound **3** unfolds the presence of Type I Cl···Cl interactions which play pivotal role towards the stability of the compound. We have further theoretically confirmed the existence and contribution of these interactions using DFT, MEP, QTAIM and NCI plot analyses. The *in vitro* antiproliferative activities of the compounds **1** and **2** have been explored in DL cancer cell lines considering MTT cell viability, apoptosis assay and molecular docking. In vitro antiproliferative evaluation of the compounds reveal that compounds **1** and **2** significantly increase cell cytotoxicity in DL cells by inducing apoptotic cell death with negligible cytotoxicity in healthy PBMC cells (8–10%). Molecular docking simulation study confirms that both compounds **1** and **2** fit well in the inhibitor binding pocket of BCL-2 family proteins (BCL-2 and BCL-XL) which are well known for the structure activity relationship of cancer growth and metastasis.

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P-178

“Degradation of e-wastes using carbohydrates in water”

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E-waste represents the fastest-growing category of global solid waste with an increment rate of 30% per annum.[1] This complex waste consists of three main components; plastic, metals (precious and regular) and glass. E-waste would be used as a source of precious metals since mining of the same is anticipated to face significant challenges in meeting future demand.[2]

Sustainable recycling of the precious metals and the plastics from e-wastes using eco-friendly processes is challenging. In order to address this issue, carbohydrates are used to extract metals from the e-wastes; mainly using their extreme complexing ability with most of the metal ions. Simultaneously, tribochemical fragmentation of the plastic components of the e-wastes are carried out. The extent of the dissolution of the metals and other components are controlled upon changing the experimental condition. For example, the extraction of Cu, Zn, and Pb ions are most effective (in the supernatant) when D-glucose and urea are used. For Sn, the highest concentration is achieved when PCBs (an e-waste fragment) are treated with D-fructose in the presence of ammonium carbonate [$(NH4)_2CO_3$]. Few more exciting results will be demonstrated during the presentation.

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P-179

Visible-light-initiated Sulfonylation of Phenylhydrazines with Thiols

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One particularly straightforward and effective way to create sulfonamides is through the sulfonylation process. Despite significant progress in constructing the sulfonamide framework, the prospective application of phenyl hydrazine as an amination source has not yet been thoroughly investigated. Here, we describe a metal-free, environmentally benign, photoredox-catalyzed thiol-based phenylhydrazine sulfonylation process using eosin Y as a photoredox catalyst and MeCN:H2O as a green solvent system. This approach demonstrates good compatibility with both aliphatic and hetero(aryl) phenylhydrazines, along with a wide range of substrates.

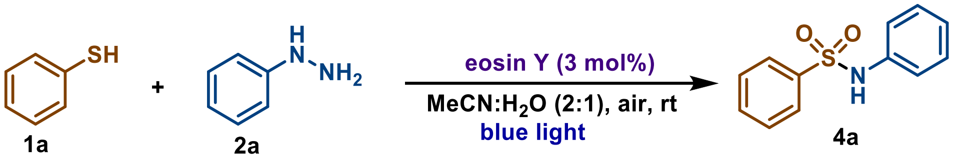

Figure 1. Visible light-mediated synthesis of sulfonamides.

Since previous methods for sulfonamide production frequently involve unnecessary steps, generate waste, and are costly, there remains a strong demand for simpler and more efficient techniques. To address this, we have developed a direct and effective method for synthesizing sulfonamides from thiols.

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P-180

Metal−Organic Framework-Supported Mono Bipyridyl−Iron Hydroxyl Catalyst for Selective Benzene Hydroxylation into Phenol

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Direct hydroxylation of benzene to phenol is more appealing in the industry for the economic and environmentally friendly phenol synthesis than the conventional cumene process. We have developed a UiO-metal−organic framework (MOF)-supported mono bipyridyl-Iron(II) hydroxyl catalyst [bpy-UiO-Fe(OH)$_2$] for the selective benzene hydroxylation into phenol using H_2O_2 as the oxidant.[1] The heterogeneous bpy-UiO-Fe(OH)$_2$ catalyst showed high activity and remarkable phenol selectivity of 99%, giving the phenol mass specific activity up to 1261 $mmol_{PhOH}\ g_{Fe}^{-1}\ h^{-1}$ at 60 °C. Bpy-UiO-Fe(OH)$_2$ is significantly more active and selective than its homogeneous counterpart, bipyridine-Fe(OH)$_2$. This enhanced catalytic activity of bpy-UiO-Fe(OH)$_2$ over its homogeneous control is attributed to the active site isolation of the bpy-Fe(OH)$_2$ moiety by the solid MOF that prevents intermolecular decomposition. Moreover, the exceptional selectivity of bpy-UiO-Fe(OH)$_2$ in benzene to phenol conversion is originated via shape-selective catalysis, where the confined reaction space within the porous UiO-MOF prevents the formation of larger overoxidized products such as hydroquinone or benzoquinone, leading to the formation of only smaller-sized phenol after monohydroxylation of benzene. Spectroscopic and controlled experiments and theoretical calculations elucidated the reaction pathway, in which the in situ generated •OH radical mediated by bpy-UiO-Fe^{II}(OH)$_2$ is the key species for benzene hydroxylation. This work underscores the significance of MOF-supported earth-abundant metal catalysts for sustainable production of fine chemicals.

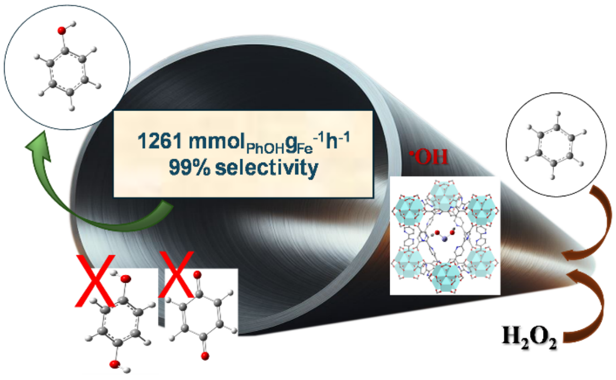

Figure 1. Graphical abstract of selective hydroxylation of benzene to phenol

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P-181

Cobalt-Catalyzed Stereospecific C-N/C-O Bond Formation of Oxiranes with Diaziridines

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Co-catalyzed stereospecific C-N and C-O bond formation of oxiranes with diaziridines has been demonstrated to furnish tetrahydro-[1,3,4]-oxadiazines under mild conditions (Figure 1).[1] Enantiomerically pure oxiranes can be coupled with high optical purities (>96% ee). High stereoselectivity, functional group tolerance, mechanistic investigation using DFT studies and natural product modification are the salient features.[2,3]

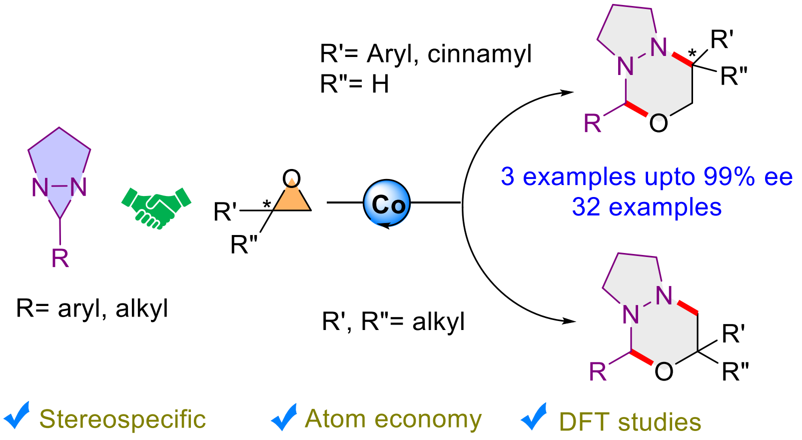

Figure 1. Stereospecific coupling of diaziridines with oxiranes

Initial optimization of the reaction conditions reveal that $CoCl_2$ is the best Lewis acid catalyst for the cycloaddition in CH_2Cl_2 solvent at room temperature. Under the optimized reaction conditions, a range of functional groups on both the substrates have shown compatibility in furnishing the desired product in moderate to good yield. Later, stereospecific transformations using optically pure oxirane yielded the intended cycloadducts in upto >99% ee.

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P-182

Nuclear targeted triazole-bridged biotin-conjugated quinoline derived Single component organic nanoparticle-based two photon-responsive Drug Delivery Systems

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Two-photon excitation (2PE) of photocaged molecules offers a promising approach for targeted therapy, as low-energy infrared (IR) light can penetrate deep into tissues while enabling noninvasive photochemistry. [1] In this study, we present a novel class of two-photon near-infrared (NIR) light-responsive, nucleus-tageted, single-component organic nanoparticle-based drug delivery systems (DDSs) utilizing triazole-bridged biotin-conjugated quinoline derivatives, synthesized via click chemistry, to selectively release the caged anticancer drug chlorambucil upon NIR irradiation at the tumor site. The biotin conjugation exploits the overexpression of biotin receptors in cancer cells, allowing for selective targeting. Notably, we also observed an enhancement in the two-photon cross-section upon the incorporation of heavy atoms into the DDSs, with values of 98, 105, and 118 GM (1 GM = 10–50 cm^4 s/photon/molecule).

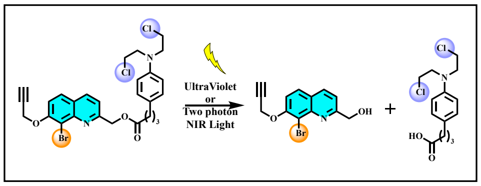

Figure 1. Graphical abstract of two photon responsive quinoline based drug delivery system

Our DDSs can be photolyzed via both conventional one-photon excitation (365 nm) and two-photon excitation (740 nm), providing precise spatial and temporal control over drug release. Upon NIR light irradiation, the two-photon-responsive system triggers controlled drug release directly within the nucleus, reducing off-target effects and improving therapeutic efficiency. The nanoparticles, synthesized using the reprecipitation technique, were thoroughly characterized through scanning electron microscopy (SEM), transmission electron microscopy (TEM), and dynamic light scattering (DLS) analyses. In vitro studies using breast cancer models demonstrated significant tumor regression, attributed to apoptotic cell death following the efficient intracellular release of the drug. Our findings highlight the potential of these DDSs in enhancing both the specificity and efficacy of cancer treatment, positioning it as a promising candidate for further preclinical and clinical evaluation.

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P-183

Tuning of Electrocatalytic Water Oxidation Activity of Cu (II) Complexes by Changing Electron Donating Nature of Ligand Frameworks

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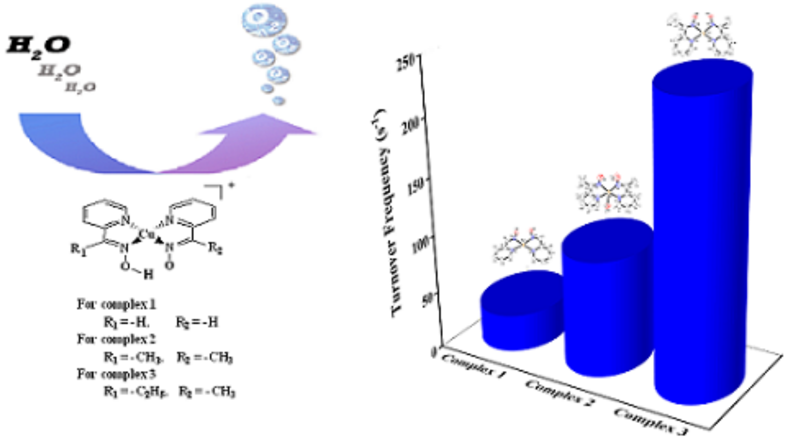
With the progress of civil society, global energy demand and environmental concerns are driving the development towards the large production of clean energy. One such sustainable alternative pathway is the production of hydrogen and oxygen through electrocatalytic water oxidation using transition metal complexes.[1-4] Therefore the development of efficient, robust, and economical water oxidation catalysts (WOC) remains a key challenge for the scientific community. Among them, copper (II)-based WOCs have been reported as competent candidates with successive improvement of catalytic activity.[5-9] In this regard, we have investigated the electrocatalytic water oxidation activity of three copper(II) complexes **1**, $[Cu(L_1H)(L_1)](ClO_4)$; **2**, $[Cu(L_2H)(L_2)(H_2O)](ClO_4)$ and **3**, $[Cu(L_3H)(L_2)](ClO_4)$ with aryl oxime ligand, L_1H, L_2H, and L_3H [L_1H = 1-(pyridin-2-yl)methanone oxime, L_2H = 1-(pyridin-2-yl)ethanone oxime and L_3H = 1-(pyridin-2-yl)propanone oxime] in neutral phosphate buffer. All three ligands have in common a pyridyl group attached to the carbon centre of the oxime moiety and differ with respect to the identity of the second substituent attached to the oxime carbon. Electrochemical investigations on the catalytic activity of complexes **1**, **2** and **3** shows that the identity of the substituent attached to the carbon center of the oxime ligand has an influence on the catalytic pathway as well as on the overall catalytic activity of the complexes.



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P-184

Regio- and stereoselective synthesis ofAllylsulfones using DABCO

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The regioselective and stereoselective synthesis of (*E*)- and *(Z)*- allylsulfones has been achieved through the reaction of Baylis-Hillman acetates with sodium salt of sulfinate in presence of 1,4-Diazabicyclo[2.2.2]octane (DABCO) and diethylether as a solvent at room temperature. The reaction proceeds via two distinct pathways: S_N2' mechanism and S_N2 mechanism. It was observed that initially (10-20 min) it predominately gives kinetically controlled S_N2 product and when the reaction time extends to 24h S_N2 substituted product completely transformed into thermodynamically controlled S_N2' substituted product.[1] Without DABCO found that it gives only S_N2' allylsulfones with 90-95% yield. The presence of DABCO can change the nucleophilic substitution at vinyl position of Baylis-Hillman acetates. The selectivity of *(E)*-and *(Z)*- isomer depends on the Baylis-Hillman acetates. Numbers of allylsulfones were synthesized using various Baylis-Hillman acetates and sulfinates with excellent yield. All the products are well characterized by Mass spectrometry, NMR and IR spectroscopy. This work shows how to synthesize stereo- and regioselective allylsulfones with gentle and effective manner, which may have uses in medicinal chemistry and chemical synthesis. [2-5]

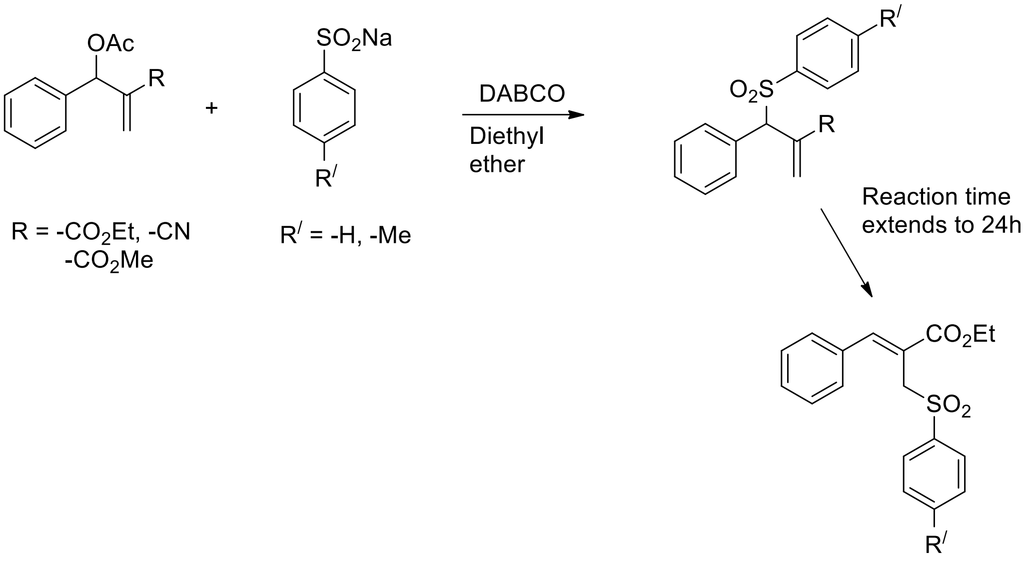

Figure 1 : Graphical abstract of synthesis of Allylsulfones.

Keywords : Stereoselective, Regioselective, DABCO, Allylsufones

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P-185

Investigation of Magnetic and Magnetocaloric Properties in disordered Spinel Compound $Fe_{2-x}Cu_xSnS_4$

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Chalcogenides have attracted considerable attention not only due to prospective applications in in thermoelectric, nonlinear optics, solar cells, superconductivity, magnetocaloric but also because of the diverse structural properties. Iron and copper-based ternary metal chalcogenides offer an extra dimension in terms of magnetism and magnetocaloric application, that makes them more intriguing. From earlier study in our group, it was observed that the magnetic properties in Mn_2SnS_4 can be tuned by suitable substitution at different sites. [1-3]

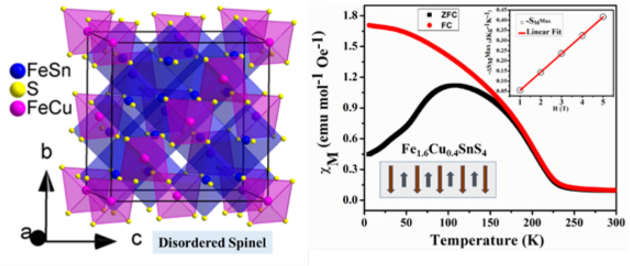

Figure 1. The disordered cubic spinel $Fe_{1.6}Cu_{0.4}SnS_4$ containing mixed valent Fe(II) and Fe(III) shows ferrimagnetic like ordering below 230 K and maximum value of $-\Delta S_m$ as 0.4 J/kg K under an applied magnetic field of 5 T.

To further understand the magnetic properties and the effect of substitution in the Fe-analogue, Fe_2SnS_4, we have studied the effect of Cu substitution on the structure and magnetic properties in $Fe_{2-x}Cu_xSnS_4$. [4] In this work we repot a detailed electronic, magnetic, structural, and thermodynamic investigation on $Fe_{2-x}Cu_xSnS_4$ using both experimental and theoretical Study. From magnetic measurements, we have observed one distinct magnetic transition at 230 K, associated with ferrimagnetic ordering which can be rationalized by taking into account the changes in the distribution of magnetic centres within the structure arising from the Cu substitution at Fe site. XPS study indicates that Fe exists in both +2 and +3 oxidation states while Cu, Sn and S adopt +1, +4 and −2 oxidation states, respectively. Magnetic susceptibility study suggests ferrimagnetic like ordering in $Fe_{1.6}Cu_{0.4}SnS_4$ below 230 K and the ordering temperature gradually decreases from 230 K to about 120 K with increase in Cu substitution. As the amount of Cu(I) increases in $Fe_{2-x}Cu_xSnS_4$, the percentage of Fe(III) increases to balance the charge. The magnetocaloric properties of polycrystalline $Fe_{1.6}Cu_{0.4}SnS_4$ has been studied for their potential applications as magnetic refrigerant at cryogenic temperatures. With an applied magnetic field of five Tesla, the maximum value of magnetic entropy change was found to be (ΔS_m) 0.4 $Jkg^{-1}K^{-1}$ with a relative cooling power (RCP) of 7 J kg^{-1}. These values are very similar to the literature reported values for Cu and Fe based compounds. Further, manipulation at the Fe site may lead to enhancement of magnetocaloric effect for practical applications.

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P-186

A multi-component synthetic route for 2-pyrazolines via acceptorless dehydrogenation of alcohols using homogeneous Ni(II) catalysts

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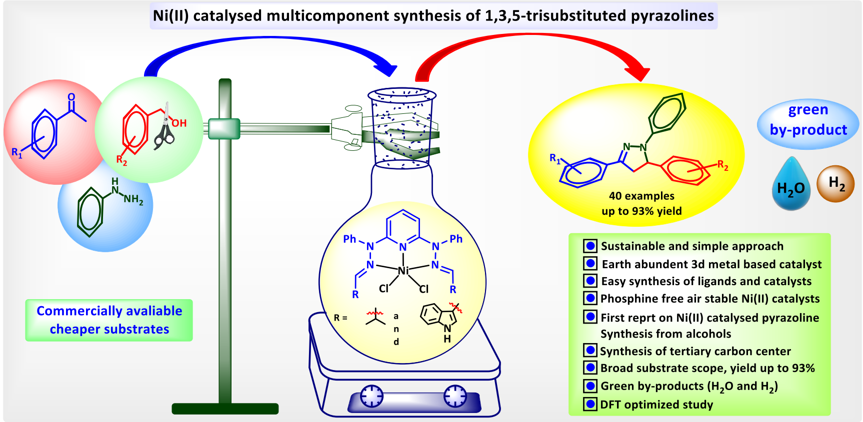
Heterocyclic compounds are a significant class of organic compounds that are widely used in modern medicinal chemistry due to their numerous applications in drug discovery and design.[1] Nitrogen-containing heterocyclic compounds accounted for more than 90% of the top 200 small molecule medicines by retail sales in 2020.[2] Among heterocyclic compounds, the pyrazole and 2-pyrazoline families belong to the five-membered heterocycles with two adjacent nitrogen atoms in their structure. Pyrazoline derivatives have been reported to exhibit versatile biological activities such as anticancer, antidepressant, antimalarial, antifungal, anti-Alzheimer's, antiparkinsonian, anti-HIV and other activities.[3] Over the last few decades, many methods have been developed for the synthesis of pyrazoles and 2-pyrazolines although several difficulties still exist in these methods such as poor selectivity, toxicity, expensive chemicals, pre-functionalization of reactants, multi-step reactions, etc.[4,5] The main challenge at the present time is to develop a cost-effective, cheaper, sustainable, and easy to handle synthetic methodology for the synthesis of five-membered N-heterocycles from commercially available substrates. In recent years, acceptor less dehydrogenation (AD) of alcohols has emerged as an efficient and greener approach to provide carbonyl compounds, which can be transformed into other extremely useful N-heterocyclic compounds.[6] In the past few years, transition metal-catalyzed multicomponent reactions have gathered a lot of interest for the production of valuable N-heterocycles. AD of renewable primary alcohols has emerged as an effective tool for synthetic organic chemists in the selective synthesis of value-added heterocyclic compounds via multicomponent one-pot methods.

Herein, we present the first efficient and sustainable multicomponent synthesis (MCS) of 2-pyrazolines using acceptor less dehydrogenation of benzyl alcohols catalyzed by nickel(II) catalysts. Two air-stable phosphine free nickel(II) complexes anchored by NNN type pincer ligands were synthesized and efficiently used in the MCS of 40 distinct pyrazoline derivatives.[7]



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P-187

Spectrophotometric Investigations of Charge Transfer Complexes formed between 1,2,4-triazoles and different acceptors: An Experimental and Theoretical Investigations

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Metal complexes of 1,2,4-triazole have gained significant interest due to their diverse structural, chemical and functional properties. These metal-triazole complexes exhibit potential applications in fields such as catalysis, molecular sensing, medicinal chemistry, and materials science. Growing interest in organic electronics, sustainable materials, and environment friendly alternatives to metal complexes drive more research into the formation of charge -transfer complexes of 1,2,4-triazoles with organic- π-molecules.

In view of this, in the present work, new charge transfer complexes of differently substituted 1,2,4- triazoles (donors) with different acceptors (DMAD, DDQ, Chloranil, TCNE etc.) have been synthesized and studied in different polarity of solvents at room temperature. The stoichiometries of the synthesized complexes were determined by the Job's method of continuous variations and found to be 1:1. The formation constant and molar extinction coefficient of the CT complexes were determined by mole-ratio method and Benesi-Hildebrand equation. The higher values of formation constant were recorded in the less polar solvent than the more polar solvent indicated the formation of a highly stable complexes. The high negative values of free energy (ΔG^0) the CT complex showed that there is strong complexation between the donor and the acceptor, which was justified by the lower value of the transition energy (Ect) obtained for the complex. The effect of different donors and the solvents on the stability and formation of charge transfer complexes have also been studied and it was found that the complexes are stable in solvent of less polarity, the bathochromic shift was also observed in the complexes.

The theoretical investigation of the synthesized charge transfer (CT) complexes were also done at the Time Dependent Density Functional Theory (TD-DFT) level using the B3LYP/6-31+G* basis set. All calculations were performed using the Gaussian16 suite of programs. The results obtained from experimental studies were found to be in close agreement with the theoretical data.

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P-188

Programmable Nano-Oscillators Engineering for Dual-State Emission in Solution and Solid Phases

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Fluorophores often lose fluorescence upon aggregation due to aggregation-caused quenching (ACQ). Dual-state emission (DSE) is a promising solution, enabling aggregation-induced emission (AIE) to maintain fluorescence even in solid states. This feature broadens their applications in biotechnology and optoelectronics[1].Here, we present an engineered fluorophore fabricated with molecular motors [2] that exhibits both AIE and DSE[3,4]. Using this dual functionality, we developed fluorescent nanowires from novel nano oscillator subunits called PCM (PAMAM dendrimer, controller molecule, and molecular motor) through electrocatalytic self-assembly. These nanowires display programmable fluorescence with broad spectra in solution and distinct cyan-green to red emission in the solid state[5].Notably, they can modulate photonic bandgaps, causing a redshift, which is promising for applications like drug delivery and infrared-sensitive technologies. These innovations pave the way for advancements in nanotechnology, optoelectronics, and light-based devices.

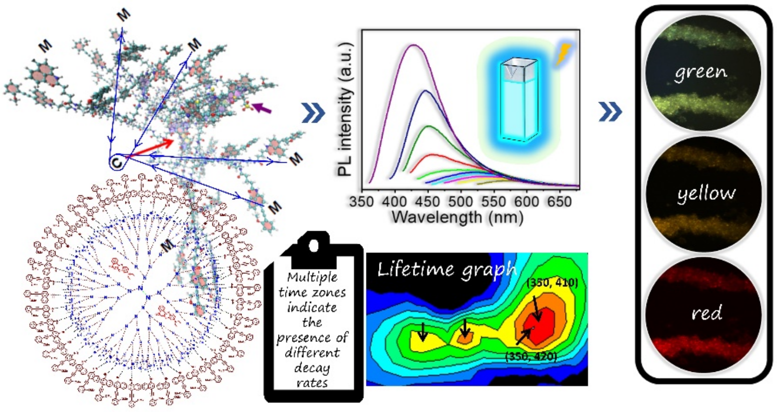

Figure 1. Pictorial Abstract of PCM oscillator that exhibits dual-state fluorescence.

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P-189

A Reusable MOF Coated Chitosan@Paper Strip Composite for Real-Time Monitoring of Pesticide Pendimethalin and Organo-Arsenic Feed Additive Roxarsone Levels in Environmental Water, Food and Vegetable Samples

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An alarming increase in the use of pesticides and organoarsenic compounds and their toxic impacts on the environment has inspired us to develop a selective and highly sensitive sensor for the detection of these pollutants. Herein, bio-friendly, low-cost Al-based luminescent metal-organic framework (1′) based fluorescent material is demonstrated that helps in sustaining water quality by rapid monitoring and quantification of a long-established pesticide (pendimethalin) and a widely employed organo-arsenic feed additive (roxarsone). The pyridine functionalized porous Al-MOF was solvothermally synthesized. After activation, it was used for fast (< 10 s) and selective turn-off detection of roxarsone and pendimethalin over other competitive analytes. This is the first MOF-based recyclable sensor for pendimethalin with a remarkably low limit of detection (LOD) (14.4 nM). Realtime effectiveness in detection of pendimethalin in various vegetable and food extracts was successfully verified. Moreover, the aqueous phase recyclable detection of roxarsone with an ultra-low detection limit (13.1 nM) makes it a potential candidate for real-time application. The detection limits for roxarsone and pendimethalin are lower than the existing luminescent materials. Furthermore, the detection of roxarsone in different environmental water and a wide pH range with a good recovery percentage was demonstrated. In addition, a cheap and bio-friendly 1′@chitosan@paper strip composite was prepared and successfully employed for the hands-on detection of pendimethalin and roxarsone. The turn-off behaviour of 1′ in the presence of pendimethalin and roxarsone was examined systematically and plausible mechanistic pathways were proposed with the help of both experimental evidence and theoretical calculations.

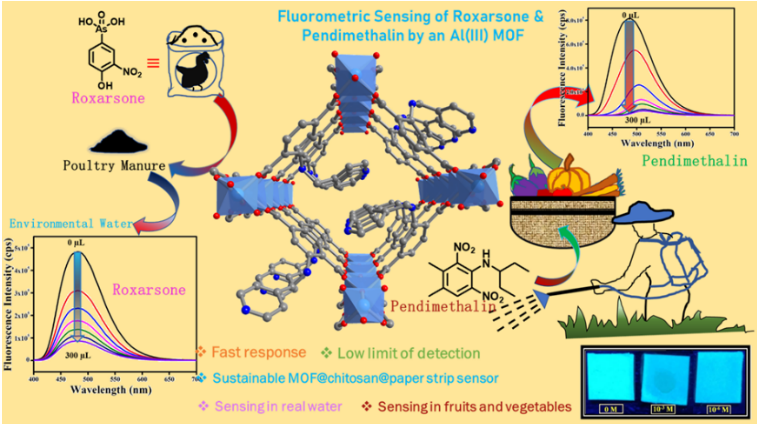

Figure 1. Graphical abstract of MOF based fluorescence sensing of Pesticide Pendimethalin and Organo-Arsenic Feed Additive Roxarsone

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P-190

Harnessing reductive BF_2-complexation *via* Ru(II)-catalyzed N–O cleavage of isoxazoles

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Developed here is a highly fluorescent organic N,O bidentate BF_2 complex from isoxazole in the presence of a Ru(II) catalyst.[1] Herein, the complexation proceeds *via* a selective N–O cleavage of the isoxazole ring. The complex shows absorption ($\lambda_{max,abs}$) in the range of 352–363 nm with an extinction coefficient (ε) in the range of 8000–64000 M^{-1} cm^{-1}, and fluorescence emission ($\lambda_{max,em}$) in the range of 413–485 nm with a Stokes shift of 61–125 nm having quantum yield up to 33%. Apart from the solution state, the solid BF_2 complex **2u** exhibits absorption at 405 nm and strong fluorescence emission at 550 nm with a quantum yield of 26.9%.

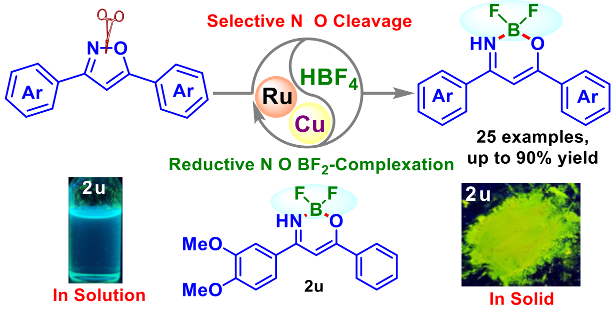

Figure 1. Ru(II)-catalyzed reductive N,O-bidentate BF_2-complexation of isoxazole *via* a selective N–O bond cleavage

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P-191

Aza Phenalenone Derivatives Using Aldrone Condensation and their Applications

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Perinaphthenone or phenalenone (PN) is a naturally occurring polycyclic aromatic hydrocarbon comprising of a ketone functional group. The moiety is found in several plants, microbial and fungal sources, and plays major role in protection of organisms against external aggressions.[1] Some of the PNs, both the naturally occurring as well as the synthetic, have demonstrated diverse range of bioactivities including antioxidant, anticancer, photo dynamic therapy, antimicrobial, and antifungal activities.[1-2] Some of the PNs have also been used as sensor for human carboxylesterase.[3] With enormous propensity to generate singlet oxygen under light irradiation, PN has established itself as a universal standard for the determination of singlet oxygen quantum yield (${}^1O_2$). The efficiency of such activities are highly rely on the nature of substitutions attached with the PN core. Accordingly, various synthetic modifications have been carried out on the PN core to tune the optical and medicinal properties.[4] Inspired by fascinating properties and wide range of applications of PNs, we aimed to bring heteroatom at the PN core and synthesize azaphenalenone derives. Using aldrone condensation, we have synthesized several different aza phenalenone derivatives and demonstrated their medicinal applications.[5]

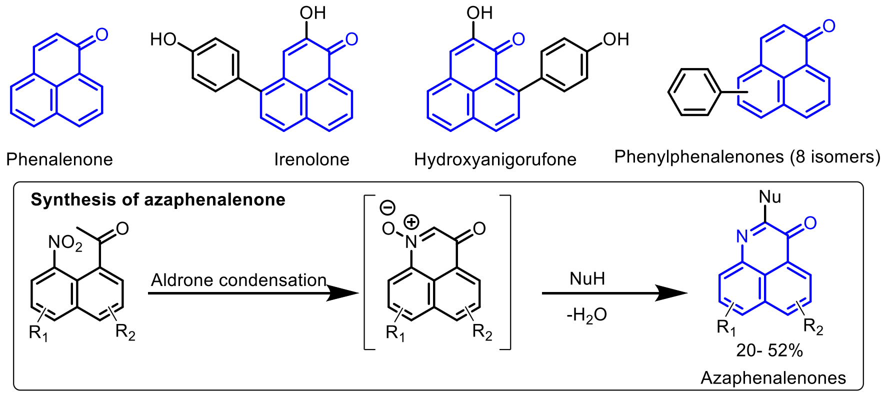

Figure 2. Structure of parent phenalenone, some of the naturally occurring and synthetically prepared phenalenones. Synthetic scheme and structure of azaphenalenones are shown inside the box.

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P-192

Enhancing C–S and C–N bond formation with ultrasound assistance: lipase-catalyzed synthesis of 2,4-disubstituted thiazole derivatives from arylethanones and thioamides

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This work presents a novel and effective synthetic procedure for 2,4-disubstituted thiazole derivatives, a class of chemicals with important biological and medicinal applications. It highlights the use of lipase as a very efficient and environmentally benign catalyst for producing thiazoles. Ultrasonic energy facilitates the reaction between aryl ethenone, $KBrO_3$, and thioamide in mild conditions. To accelerate the reaction and increase product yields, ultrasound irradiation is used. This article describes a lipase-catalyzed, ultrasound-assisted synthesis that is more environmentally friendly and sustainable than traditional techniques. It has potential uses in medicinal chemistry and drug development. This strategy could improve thiazole synthesis and lead to more effective and sustainable chemical processes.

Figure 1. Graphical abstract for the synthesis of 2,4-disubstituted thiazole under ultrasound.

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P-193

Surface-Engineering of $CaTiO_3$ for Photocatalytic Hydrogen Evolution Reaction through Enhanced Oxygen Vacancy

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Surface engineering has been an important strategy in attaining a higher catalytic activity in comparison with pristine samples. $CaTiO_3$ is a well-known photoactive material but lacks photo-to-electron conversion efficiency. Herein, we demonstrate a simple path-way that could achieve a higher surface area, active site exposure, and oxygen vacancies. The experimental results using different concentrations of HNO_3 illustrated the selective leaching of Ca(II) ions, which leads to the partial conversion of Ti^{4+} to Ti^{3+} and the formation of oxygen vacancy. This eventually resulted in an engineered electronic state that modifies the band alignment and improves the charge transfer and migration rate. The optimized photocatalyst (CTO-5) exhibits approximately six times enhanced hydrogen evolution rate of 58.1 $\mu mol \cdot g^{-1} \cdot h^{-1}$ than the pristine $CaTiO_3$ (8.7 $\mu mol \cdot g^{-1} \cdot h^{-1}$). Our work offers new intuitions into the rational design of photocatalysts with surface-engineering methodology without using any noble metal.

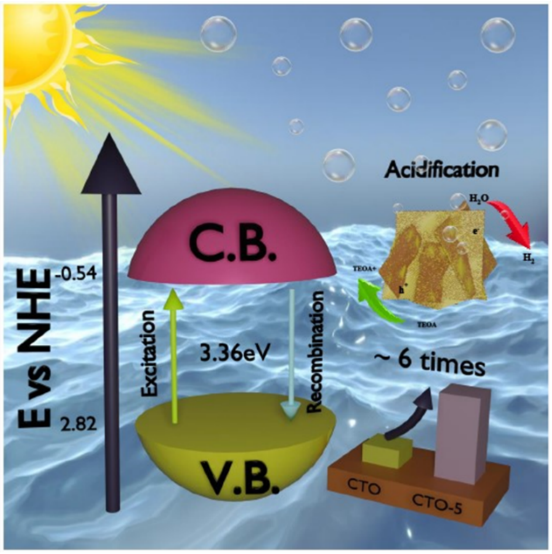

Figure 1 Graphical abstract of Surface-Engineering of $CaTiO_3$ for Photocatalytic Hydrogen Evolution

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P-194

Time-Encoded Information Encryption with pH Clock Guided Broad-Spectrum Emission by Dynamic Assemblies

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The development of anti-counterfeiting strategies and message encryption methods has drawn tremendous attention in the last decade. Fluorescence-based encryption from aggregation-induced emission (AIE) derived smart materials solves the problems to an appreciable extent. However, installing multiple features like hierarchical security levels, orthogonal decryption, stimuli-specific decoding, and temporal dynamicity all in a single encryption routine is still challenging. To address this complication, a pH-switchable fluorescent assembly of a cyanostilbene (CSB) AIEgen derivative and an aliphatic acid, myristic acid, has been implemented in this study. Primarily, the pH responsiveness and reversibility in the fluorescence properties of the pH-controlled co-assembly were experimentally demonstrated. pH-dependent morphologies and different emission colors could be isolated. Further, a TRIS: Glucanolactone (GdL) triggered pH clock was employed. This generated a temporally regulated dynamic pH in the solution of the assembling molecules. Time-dependent experiments were conducted for the analysis of the pH-clock instructed co-assembly and emissive changes. Additionally, for the first time we have monitored the lifetime and quantum yields under dynamic conditions. Concomitantly, a pH clock guided time-programmed transitory multicolor emission was executed, which passed through a transient white light zone. Furthermore, smart multi-input fluorescent chemical AND gates were constructed with the aid of the pH-specific emission. The AIEgen attributes of the CSB molecule alone served as a useful on-paper secure anti-counterfeiting ink with UV light-specific decryption. Later, an intelligent multi-dimensional secure data encryption method was realized where the fourth dimension is introduced in the form of time. The anti-counterfeiting strategy offered time-locked features, hierarchical levels, and orthogonal condition-specific decryptable qualities.

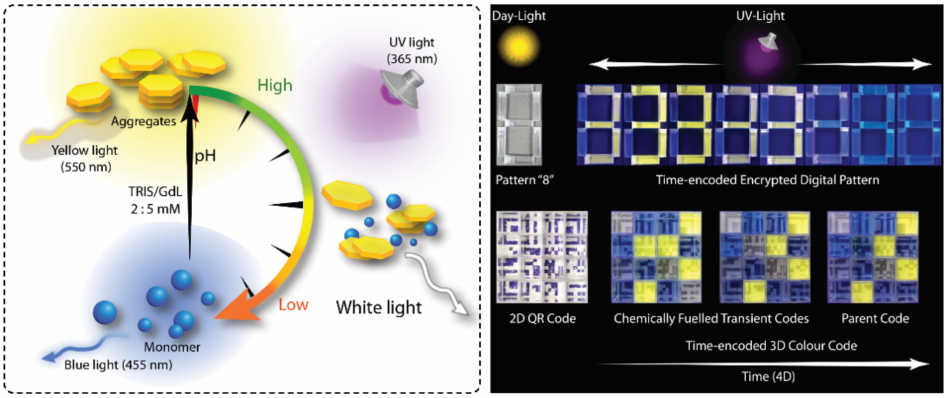

Figure 1. Graphical abstract of pH clock guided transitory emission in dynamic assemblies and 4D information encryption

Keywords: Transient Assembly, pH clock, White light, Anit counterfeiting

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P-195

Frustrated Ion Pair Interactions Driven Anion Assisted Concerted Addition of Ketoximes/Aldoximes and Hydroxamic Acids to Glycals

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N-O linked glycosides exhibit diverse pharmaceutical and biological activities. Moreover, their heightened enzymatic stability makes them intriguing structural mimics of natural glycosides, capturing the interest of researchers.[1] In natural antitumor antibiotics, compounds such as esperamicins A and calicheamicins showcase N-O linked oligosaccharides.[2] These unique linkages play a pivotal role in controlling the conformation of the molecules, ensuring the selective binding mode to specific DNA sequences.[3] Additionally, the ease of preparation and stability of oximes have led to the widespread adoption of the aminooxy group as a distinctive linker for connecting various biomolecules.[4] Oximes and hydroxylamides are notable for their role as coupling partners in organic synthesis. However, their direct application as acceptors in *O*-glycosylation with glycal donors remains largely unexplored.

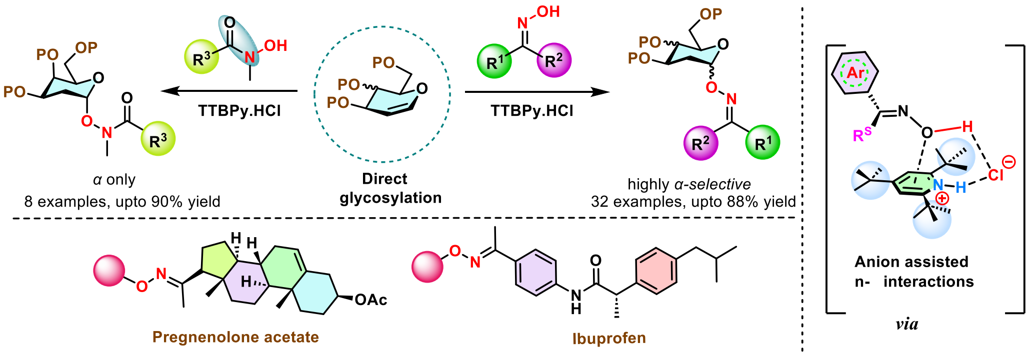

Figure 1. Synthesis of 2-Deoxy N-O linked Glycosides

Herein, we introduce a novel 2-deoxy glycosylation method for synthesizing N-O linked glycosides facilitated by sterically strained 2,4,6-tri-*tert*-butylpyridinium salts. This approach offers a broad substrate range, high tolerance for functional groups, and easy scalability, resulting in glycosyl oximes and glycosyloxyamines with exclusive *α*-selectivity and retention of E/Z geometries with excellent yields. The effectiveness of this method is showcased through site-selective functionalization of glycosylated products, late-stage modification of bioactive drug molecules and disaccharide synthesis. This innovative strategy offers an alternative route and holds promise for wide-ranging applications in the construction of bioactive N-O linked glycosides in the future.

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P-196

Improving the electrocatalytic activity of NiTe nanoflakes by coupling CeO_2 for oxygen evolution reaction

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Transition metal tellurides have garnered significant attention as potential alternative electrocatalysts for the oxygen evolution reaction (OER) due to their high electrical conductivity and diverse phases and compositions. However, their catalytic performance is hindered by limited active site exposure and suboptimal adsorption energies of oxygenated intermediates, resulting in relatively low catalytic activity.[1] CeO_2 is a very impressive catalyst due to its unique reversible Ce^{3+} and Ce^{4+} oxidation states and intrinsic oxygen vacancy defects, which can supply and withdraw electrons that facilitate the electrochemical reaction. Additionally, CeO_2 possesses dominant mechanical resistance, anticorrosion activity, and remarkable redox property, which are highly desirable properties of an electrocatalyst.[2] Herein, a hetero-structure of CeO_2 decorated NiTe nanoflakes are constructed on a nickel foam scaffold (denoted as NiTe/CeO_2@NF) through a facile two step hydrothermal method. Accordingly, the as-developed NiTe/CeO_2@NF exhibits an excellent electrocatalytic performance for the OER with a low overpotential of 273 mV at a current density of 10 mA cm^{-2} in 1.0 M KOH with a Tafel slope value of 81mV dec^{-1} . The composite shows a remarkable stability of 40 hours in the harsh alkaline medium.

Figure 1. Schematic representation of the synthetic protocol used for the fabrication of NiTe/CeO_2@NF

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P-197

VALORISATION OF RICE STRAW INTO A VALUABLE PIGMENT: PRODIGIOSIN

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Prodigiosin, a tripyrrole microbial pigment is obtained from many bacteria, like *Serratia marcescens.* It is a red colour pigment that could be a potential replacement for synthetic dyes. It has been reported to exhibit anti-fungal, anti-bacterial, anti-metastatic, anti-proliferative, and immunosuppressive properties. Therefore, it has a great demand in various industries, including food, cosmetics, and nutraceuticals, as a natural alternative to synthetic colorants. Prodigiosin, with extensive applications in various fields, has challenges due to its expensive production process, limited accessibility, and modest yield. To address this problem, the present study focused on the cultivation of naturally isolated *Serratia marcescens* CMS2 and optimizing prodigiosin production at lab scale and then further scaling upto pilot scale. This study made use of rice straw-derived xylose as an economical source of carbon. Peanut de- oiled cake was used to enrich the cost-effective growth, prodigiosin production was amplified by a stunning 1.9 times. After optimizing conditions for production pH (7), substrate concentration (1.5%), inoculum size (1.25%), and agitation rate (200 rpm), 0.5048 colour value units per mg of prodigiosin were obtained. After purification using column chromatography, various analytical techniques are used for characterization, like UV-vis spectroscopy, UPLC chromatography, and TLC chromatography. The UV-visible spectra revealed a prominent 535 nm absorption peak. After optimizing every parameter, prodigiosin could be an economically viable option that can be used for different types of applications. In the future, our study will focus on forming a biodegradable biofilm using prodigiosin that could be used for food packaging.

Keywords: Prodigiosin, Column chromatography, Rice straw, Microbial pigment.

P-198

ROP of Quinazolinones to Polyacylamidines using a Cesium Catalyst

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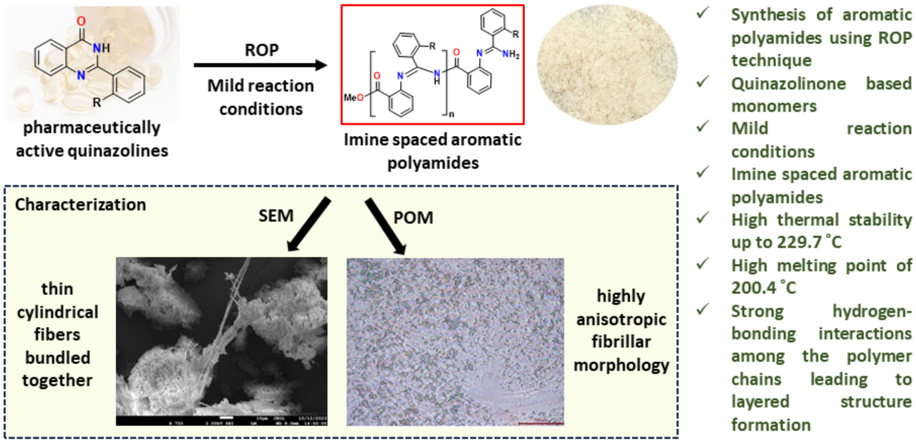
In this work, we have reported ring-opening polymerization of quinazolinones to produce novel polyacrylamides, led by a unique cooperation between a cesium metal centre and imino-phosphanamidinate ligand. The polymers were characterized using ^{1}H, ^{13}C, HSQC NMR, GPC, DSC, TGA, and PXRD. The morphological studies revealed the formation of a unique macromolecular assembly producing nanofibers without a templating agent with excellent control of molecular weights and polydispersity index.



- ✓ Synthesis of aromatic polyamides using ROP technique
- ✓ Quinazolinone based monomers
- ✓ Mild reaction conditions
- ✓ Imine spaced aromatic polyamides
- ✓ High thermal stability up to 229.7 °C
- ✓ High melting point of 200.4 °C
- ✓ Strong hydrogen-bonding interactions among the polymer chains leading to layered structure formation

Figure 1. ROP of quinazolinones to polyacylamidines

Quinazolinones obtained were used as monomers in the ring-opening polymerization (ROP) in the presence of Cs catalyst. These novel polyacylamidines display a highly crystalline behavior with a distinct Tg value close to 200 ^{O}C and thermal stability up to 250 ^{O}C. The Cs catalyst has previously been reported by our group in the ROP and ring-opening copolymerization (ROCOP) of cyclic esters.[1]

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P-199

Janus nanoparticles for enhanced cell uptake and drug delivery

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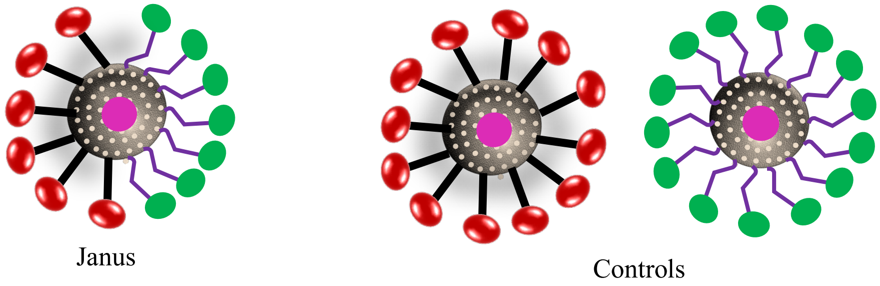
Colloidal Janus nanoparticles exhibit unique properties that make them suitable for a wide range of applications. They can serve as micro/nanomotors,[1] emulsion stabilizers, drug delivery carriers,[2] multifunctional theranostic agents and offers enhanced performance in various fields. Although colloidal Janus nanoparticles have significant biomedical application potential, their interaction with cells has been relatively less studied. Here we have demonstrated 50-100 nm porous Janus particle for enhanced cellular interaction and uptake due to Janus functionalization.[3] These Janus nanoparticles are asymmetrically terminated with two different functional groups such as arginine-dextran, urease-dextran and decylamine-dextran. The porous structure of the nanoparticles is used for the loading of small-molecule drugs and then for enhanced cell delivery of drugs with enhanced therapeutic performance.



Janus

Controls

Figure 1. Schematic represntation of Janus and control nanoparticles.Here green circle represents dextran and red circle represents arginine/urease/decylamine.

Results suggest that Janus nanoparticles with anisotropic functionalization have a wide range of biomedical application potentials that are yet to be explored. This includes the cellular uptake of smaller sized (less than 20 nm) Janus nanoparticle, drug delivery applications of urease conjugated Janus nanoparticles-based nanomotors etc.

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P-200

CeO_2-Mn_3O_4 Solid Solutions: Efficient Photocatalyst towards Degradation of Phenolic Compounds

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Most of the phenolic pollutants degradation studies employing Mn_3O_4 have been reported using peroxymonosulphate (PMS) activation, airflow or ozone oxidation [1-4]. To the best of our knowledge, hausmannite (Mn_3O_4), a potent photocatalyst, has not been studied properly towards photocatalytic degradation of phenolic compounds, and so for Mn_3O_4-CeO_2 solid solutions. Hence, we felt the urge to develop earth abundant, nontoxic, environmentally benign Mn-Ce oxide-based photocatalyst that can efficiently work towards phenolic pollutants photodegradation without using PMS activation, airflow or ozone oxidation.

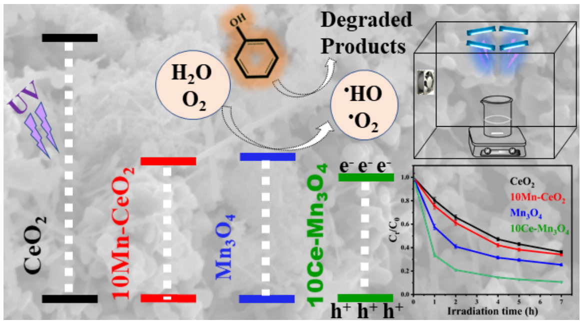

Figure 1. Graphical abstract of phenol photocatalytic degradation using CeO_2-Mn_3O_4 solid solutions.

In the present study, Mn_3O_4, CeO_2 and their two solid solutions ($10Ce$-Mn_3O_4 and $10Mn$-CeO_2), synthesized by means of co-precipitation method, are investigated for UV-light driven photocatalytic degradation of phenolic compounds. The two substituted nanocatalysts $10Ce$-Mn_3O_4 and $10Mn$-CeO_2, possess higher surface area, reduced band gap and distorted coordination environments compared to bare Mn_3O_4 and CeO_2, respectively, as indicated by Rietveld refinement of PXRD data, BET, UV and Raman analysis. $10Ce$-Mn_3O_4 shows the best catalytic activity towards phenol degradation, which has been optimized to achieve promising performance of about 89.3% phenol degradation in 7 h UV irradiation at pH 3, 0.27 g L^{-1} catalyst dosage and 25 ppm initial phenol concentration. Density of state (DOS) calculations support the observed catalytic activity trends, which show that on hetero atom substitution, band gaps of $10Ce$-Mn_3O_4 and $10Mn$-CeO_2 reduce owing to the incorporation of new energy level at the interband region. Superoxide radicals (${}^{\bullet}O_2^{-}$) and holes (h^+) mainly take part to degrade the phenol pollutants confirmed from the scavenging study. $10Ce$-Mn_3O_4 exhibits promising activity retention up to the fifth recycle. $10Ce$-Mn_3O_4 is also tested for photodegradation 2,4-dichloro phenol (2,4-DCP), which shows very high degradation efficiency of 97.5%. Thus, this study shows the potential of $10Ce$-Mn_3O_4 as an earth abundant, nontoxic and environmentally benign photocatalyst for organic pollutants degradation and further can be useful for industrial wastewater treatments in future

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P-201

Photoenhanced intrinsic peroxidase-like activity of metal free biocompatible borophene photonanozyme for colorimetric sensor assay of dopamine biomolecule

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Borophene, a monoelemental 2D structured boron sheet similar to graphene, has garnered interest in recent times due to their unique physicochemical properties such as high structural anisotropy, optical transparency, excellent mechanical compliance, high thermal conductivity, and high electron mobility.[1-4] Owing to these outstanding properties, BNSs have emerged as a promising candidate for a wide range of applications, from optoelectronics and nanoelectronics to catalysis and biosensing.

In 2018, Li et al. utilized liquid-phase exfoliation (LPE) for the first time using IPA as solvent.[5] Later in 2019, exfoliation of boron using water as a solvent for 24 hours to produce freestanding borophene was first reported by Ranjan et al.[6] Herein, we have adopted the LPE method with water as a solvent to produce biocompatible borophene nanosheets exhibiting enzyme-like properties. We used low-power probe sonication to produce borophene nanosheets from bulk boron powder within a much lower time with the help of pre-treatment of boron powder using ball-milling. The synthesized borophene was then established as a photonanozyme for the first time that exhibited excellent peroxidase-like activity towards the oxidation of a chromogenic substrate 3,3′,5,5′-tetramethylbenzidine (TMB). The photo-enhanced peroxidase-like activity of borophene photonanozyme is due to the comparable band gap energy with the visible light. A nanozyme-based colorimetric sensor assay was developed using borophene photonanozyme for the detection of an important biomarker dopamine (DA) based on the ability of DA to inhibit TMB oxidation. The developed sensor assay was capable of detecting DA selectively and sensitively, thus enabling the detection of DA in different biological fluids.

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P-202

Designing of Anthraquinone based flexible dicarboxylic acid[3-(carboxymethoxy)-9,10—dioxo-9,10-dihydro-anthracen-2yl]glycine and desingning co-crystal.

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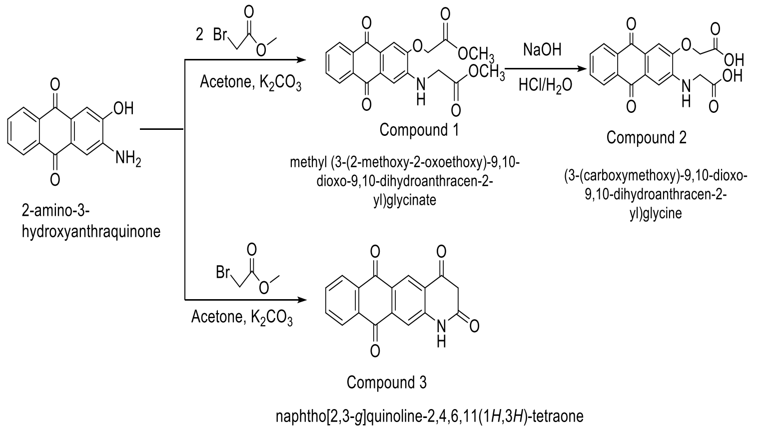
In this study, the synthesis of new anthraquinone-based flexible carboxylate ligand, [3-(carboxymethoxy)-9,10-dihydro-anthracen-2-yl]glycine (compound 2) from reaction of 2-amino 3-hydroxy anthraquinone and methylbromoacetate in dry acetone, is described and the structural details have been confirmed by using FTIR, UV, NMR and X-Ray crystallographic techniques. The interesting fact is that the end product can be varied on varying the ratio of the reactant as depicted in Scheme 1, when the reaction is carried out in the stoichiometric rattio 1:1, it results in the formation of a cyclization product. The complexation properties of Compound 2 will be studied by designing redox active metal organic frameworks and co-crystalization with nitogen containing ligands such as pyridine, 2,2' bipyridyl, 4,4' bipyridyl as anthraquinone based co-crystals. It has numerous beneficial applications on removing pollutants like dibenzothiophene and 4,6-dimethyldibenzothiophene in gasoline and diesel fuels, which cannot be removed by conventional desulfurization technology [1]. MOFs based on anthraquinone systems are known to show electroactive properties[2], PCET[3] and flourescence activity[4].



Scheme 1: Synthesis of dicarboxylic acid [3-(Carboxymethoxy)-9,10-dioxo-9,10-dihydroanthracen-2-yl] glycine ,compound 2.

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P-203

Direct Stereoselective Synthesis of 2-Deoxyglycosides via Visible-Light Induced Photoacid Catalyzed Activation of Glycosyl o-[1-(p-MeO-Phenyl)vinyl]benzoates (PMPVB) as Donors

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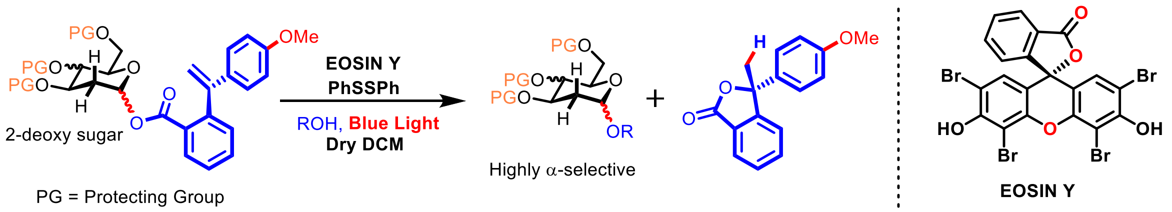
2-Deoxysugars have been part of many natural products and these are molecules of significant biological interest and have shown antibiotic and anticancer activities.[1] Studies of modifying the oligosaccharides with insertion of 2-deoxysugar moieties have found to significantly alter the biological activity of the compounds.[2] Also, stereoselective 2-deoxyglycosylation remains one of the challenging classes of glycosylation reactions due to the lack of any stereo-directing group at C-2 position and hence one has to rely on other factors like protecting group manipulations, to achieve high selectivities.3 Owing to their importance, this particular class of compounds have received considerable interest from carbohydrate community over the past few decades and has resulted in the developed of numerous interesting methods for the synthesis of 2-deoxyglycosides. Despite the developments, it is important to have new methods that are in contrast or complement the existing ones.



- Photoacid catalytisis
- Remote activation
- Stable yet reactive 2-deoxy donors
- Recyclable leaving group
- -selective glycosylation
- 28 examples.

Figure 1. Visible-Light Induced Photoacid Catalyzed Activation of PMPVB donors.

Herein, we presenting photoacid catalyzed synthesis of 2-deoxy glycosides using the stable glycosyl PMPVB donors employing the Eosin Y and PhSSPh catalytic system in the presence of blue-LED lights. The glycosyl PMPVB donor activation is achieved by the remote activation of alkene functionality under the photoacid catalysis followed by a 5-exo-trig cyclization leading to the glycosyl oxocarbenium ion that was trapped to provide the glycosyl products in excellent yields and decent selectivities under mild conditions. These mild photoacid conditions also allow the selective activation of 2-deoxy PMPVB donors in the presence of 2-oxydonors that can be useful in oligosaccharide synthesis. This method is also useful towards the photoacid catalyzed synthesis of *p*-methoxybenzyl-alkyl ethers. A variety of protecting groups are tolerated under these mild photocatalytic conditions. A range of sugar donors and acceptors underwent facile coupling to provide the glycosyl products.

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P-204

Stimuli-responsive biotin-anchored prodrug for targeted delivery of anti-cancer agent NBDHEX with turn-on NIR fluorescence

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Glutathione S-transferases (GSTs) are enzymes that catalyze the conjugation of glutathione (GSH) with a range of electrophilic bioanalytes.[1] Notably, GSTP1 is highly overexpressed in various organ-specific cancer cells in contrast to the normal cells.[2] It serves as a prognostic indicator and is associated with chemoresistance in breast cancer patients.[3] Interestingly, NBDHEX is reported to be a selective and a suicide inhibitor of GSTP1 endowed with outstanding anticancer activity in different tumor models.[4]

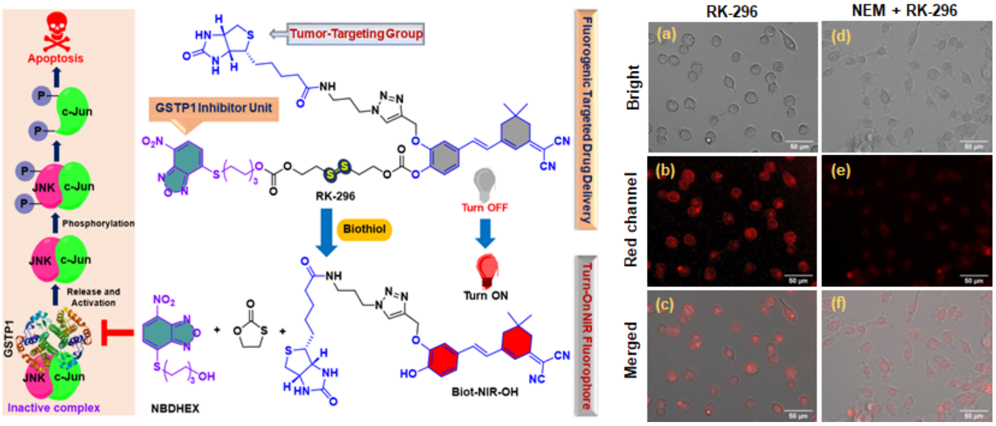

Figure 1. Schematic representation of the biothiol-triggered activation of the prodrug.

Therefore, biothiol-activatable prodrug **RK-296** was rationally developed using multi-step organic synthesis for the targeted delivery of the potent anti-cancer agent NBDHEX with concomitant turn-on near infrared (NIR) fluorescence (**Figure 1**). Moreover, the prodrug **RK-296** was anchored with the cancer cell-targeting biotin moiety for enhancing the selectivity of the designed prodrug towards cancer cells over the normal cells. Activation of the prodrug by the intracellular biothiols such as reduced glutathione (GSH) was confirmed as evidenced by the intense red emission under the fluorescence microscopy and the potent anti-proliferative activity of the released NBDHEX in the cellular medium. Therefore, the outcome of the study with the sustained release of NBDHEX from the prodrug would be useful in ameliorating the off-target side-effects of NBDHEX.[5]

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P-205

Self-assembled photosensitizer as photo-switchable oxidase mimic

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Nanozymes, which are nanomaterials with enzyme-like catalytic properties, have garnered significant attention due to their ease of synthesis, cost efficiency, high stability, robust catalytic performance, and adaptability [1]. Light-activated nanozymes are particularly notable for their ability to precisely regulate catalytic activities through light exposure, making them ideal for applications such as photodynamic therapy, biosensing, and controlled drug delivery [2]. However, many current methods for synthesizing nanozymes involve toxic solvents, extreme conditions, or complex procedures, which limit their large-scale production and practical applications.

This study investigates the potential of light-sensitive supramolecular polymers as advanced nanozymes. By synthesizing an innovative photosensitizer that exhibits aggregation-induced emission [3] and oxidase mimic activity, the study leverages supramolecular interactions to fine-tune catalytic performance. This nanozyme uses dioxygen as an oxidant, eliminating the need for harmful H_2O_2, and its activity can be easily controlled by light. We studied the influence of supramolecular interactions on the aggregation behaviour. By modifying the functionality of the molecules to adjust their degree of aggregation, assemblies with extended lifetimes were achieved, leading to sustained reactive oxygen species (ROS) generation and enhanced oxidase activity. The findings demonstrate that the supramolecular aggregation of the photosensitizer directly affects the intensity of ROS generation, providing precise control over the nanozyme's catalytic activity. This research paves the way for the design of highly efficient, biocompatible, metal-free, light-sensitive supramolecular nanozymes with promising applications. The fabricated nanozyme has been utilized for antibacterial activity against gram-positive and gram-negative bacteria.

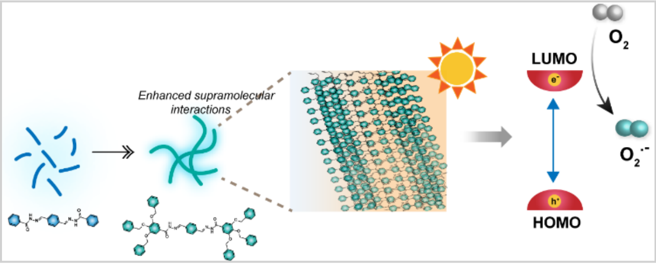

Figure 1. Graphical abstract of the photo-switchable oxidase mimetic nanozyme

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P-206

Design of Ceria Nanoparticles Decorated MXene Photocatalysts to Drive Selective and Efficient Photoreduction of CO_2 to Ethanol

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Climate change has prompted scientists to search for possible ways of reducing CO_2 emissions or even capturing it from the atmosphere. Photocatalytic CO_2 reduction has emerged as a promising strategy, capitalizing on solar energy to drive the conversion of CO_2 into valuable products.[1,2] **CeO_2**, a metal oxide is a promising material for designing highly active catalyst for the photoreduction of carbon dioxide (CO_2RR). It is one of the most studied metal oxide-based photocatalysts owing to its greater thermal stability, nontoxic nature and due to the redox-active nature of the Ce ion and the capability to switch the oxidation states from Ce^{3+} to Ce^{4+} while exposed to light, it shows efficient photocatalytic activities due to the presence of oxygen vacancies in the **CeO_2**. Herein, **CeO_2/Ti_3C_2 MXene** hetero-structured photocatalysts have been synthesized hydrothermally that exhibit superior CO_2 reduction to ethanol and methane. The intimate interfacial interactions between **CeO_2** and **Ti_3C_2MXene**, can lead to improved charge separation, faster charge transfer kinetics, and an increased degree of surface sites for CO_2 absorption and activation, in the **Ti_3C_2 MXene/CeO_2** heterostructure photocatalysts. In order to optimize the photocatalytic CO_2 reduction efficiency, **Ti_3C_2 MXene** loading amount has been varied and the optimized **5-TC/Ce** shows CO_2 reduction with a drastically enhanced yield of ethanol of the order of 6127 $\mu molg^{-1}$ at 5h with 98% selectivity and 7.54% apparent quantum efficiency, which is 6 folds higher than that of ethanol produced by the bare **CeO_2**.[3]

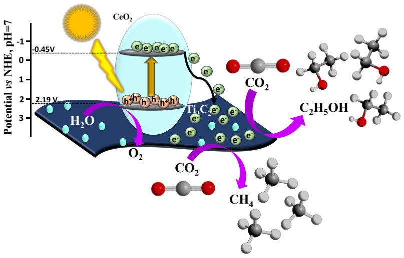

Figure 1. a) Plausible Mechanism of photocatalytic CO_2 reduction with **CeO_2** and **Ti_3C_2 MXene**

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P-207

Designing Cobalt(II) Complexes for Tandem Dehydrogenative Synthesis of Quinoline and Quinazoline Derivatives

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Saturated and unsaturated N-heterocyclic compounds are highly appealing and emergent structural scaffolds as they frequently appear as key structural units in several life-saving drugs which aim to treat a variety of medical issues.[1] Such privileged scaffolds are ubiquitous in various natural products, agrochemicals, pharmaceuticals as well as bulk and fine chemicals.[2] Owing to its growing impetus and profound applications, the development of concise, efficient and greener protocols to synthesize these N-heterocyclic scaffolds directly from renewable and widely available starting materials is very enticing.[3] In this perspective, acceptorless dehydrogenation (AD) and borrowing hydrogen catalysis have become an elegant toolbox for the benign construction of these intricate molecular scaffolds; where only H_2 and/or H_2O are liberated as nontoxic byproducts.[4] The precious noble metal-based catalytic system has advanced significantly in recent decades.[5] However, environmental and economic pressure has confined the continual use of noble metals in homogeneous catalysis. Thus, recent years have witnessed an exigency for developing new and efficient base metal catalysts for useful organic transformations.[6] In this regard cobalt complex catalysed reactions have gained unwavering attention because of their lower toxicity and diverse electronic structural behaviour, substitutional lability and ability to adopt different coordination geometry, which offers unique selectivity and reactivity patterns.[7]

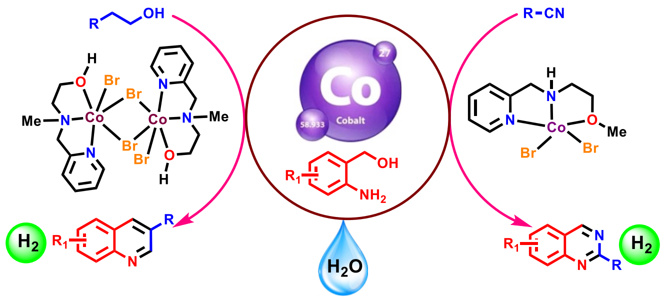

Figure 1. Graphical representation of Co-catalysed tandem dehydrogenative synthesis of Quinoline and Quinazoline derivatives

Herein, we have constructed three new Co(II) complexes in which steric features governed their structural geometry. The metal ligand-cooperation behaviour of the alkoxy arm is utilized to explore the catalytic activities of these complexes towards dehydrogenation. A wide range of C-3-substituted quinoline and quinazoline derivatives were synthesized in high yields. The developed protocol's usefulness is enhanced by the chemoselective transformation of different fatty alcohols to synthesize heterocycles having distal unsaturation. Various kinetic, mechanistic, and control studies were conducted to comprehend the reaction route.

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P-208

D-A-D-based Dinuclear Tridentate Ru(II) Complex with Strong Near-Infrared Light-Triggered Anticancer Activity

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Light-based photocatalytic cancer therapy (PCT) has emerged as a new non-invasive cancer treatment to overcome drug resistance problems with minimal side effects.[1,2] Most of the reported metal-based complexes can only be activated by blue or green light, limiting the tissue penetration depth of light-cased cancer therapies.[2,3] So far, the mainly extended conjugation in ligands approach has been used to red-shift the adsorption, but the molar absorption coefficient has still been extremely low.[1,4,5] Herein, we present a novel dinuclear Ru(II) complex, absorbing **RuX**, featuring a donor-acceptor-donor (D-A-D) linker, absorbing near-infrared (NIR) region light.[6] It is worth mentioning that it represents the first example of a bis-tridentate polypyridyl Ru(II) complex-based photocatalytic anticancer agent with strong absorption around 700 nm in the NIR region with NIR phosphorescence with λ_{em} *ca.* 800 nm.[6] **RuX** displayed both type-I and type-II reactive oxygen species (ROS) generation indicating its high potential as a photo-activated anticancer agent (Figure 1). In addition to producing different ROS, **RuX** also exhibited impressive photo-oxidation of amino acids, NADH, and NAD(P)H, making it an effective anticancer treatment for both hypoxia and normoxia tumors (Figure 1).[6] Mitochondria localizing **Rux** displayed remarkable photocytotoxicity (IC_{50} = 0.66 μM) upon 700 nm NIR light irradiation with photocytotoxicity index (PI = IC_{50}(dark)/IC_{50}(light)) > 100 against 4T1 cell line. Encouragingly, **RuX** also exhibited photo-cytotoxicity (IC_{50} = 3.73 μM) with a PI over 10.[6] **RuX** is the first Ru(II)-based photosensitizer with strong NIR LED light-triggered anticancer activity under hypoxic conditions representing a breakthrough in the search for a photocatalyst showing deep tissue penetration, high molar extinction coefficient, and excellent therapeutic effect.

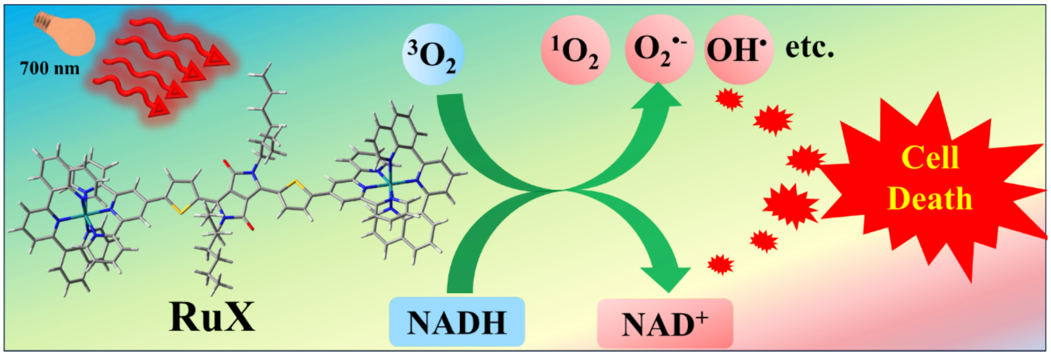

Figure 1. Schematic representation of anticancer activity of **RuX** under NIR-light irradiation.

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P-209

Design And Synthesis of a POD-mimicking Bionanozyme as Colorimetric Probe for Neurotransmitter Detection

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Peroxidases, a group of oxidoreductase enzymes, are widely employed for various biotechnological applications, but their inherent limitations-including high production costs, instability, and challenges in recovery-have restricted their broader utilization.[1] To overcome these constraints, the de novo design of synthetic enzymes has emerged as a promising strategy. In this study, we report the design and synthesis of a peroxidase (POD) mimicking bionanozyme, represented as Cu-L (where L is a biomolecular ligand). The synthesized Cu-L bionanozyme demonstrated enhanced stability under extreme pH and temperature conditions.[2] The Cu-L was characterized using various analytical techniques, including UV-Visible, HR-SEM, HR-TEM, PXRD, FT-IR, and XPS. To evaluate the POD-like activity of Cu-L, substrate-dependent kinetic studies were performed, and kinetic parameters were determined using the Michaelis-Menten model. The kinetic analysis revealed superior catalytic efficiency for the Cu-L, with a maximum velocity (Vmax) of 50.62 nM sec^{-1} and a Michaelis constant (Km) of 0.794 mM, indicating better performance compared to natural peroxidases. Furthermore, the Cu-L bionanozyme was employed for the colorimetric detection of the neurotransmitter dopamine (DA). The calculated limit of detection (LOD) for DA was 0.267 µM, which is significantly lower than previously reported values, demonstrating the high sensitivity of Cu-L for DA detection.[3] Finally, to assess the therapeutic potential of the synthetic peroxidase, in vivo anticancer studies will be conduct. This work highlights the development of a biomolecule-based synthetic biocatalyst with dual applications as a biosensor and a potential therapeutic agent.

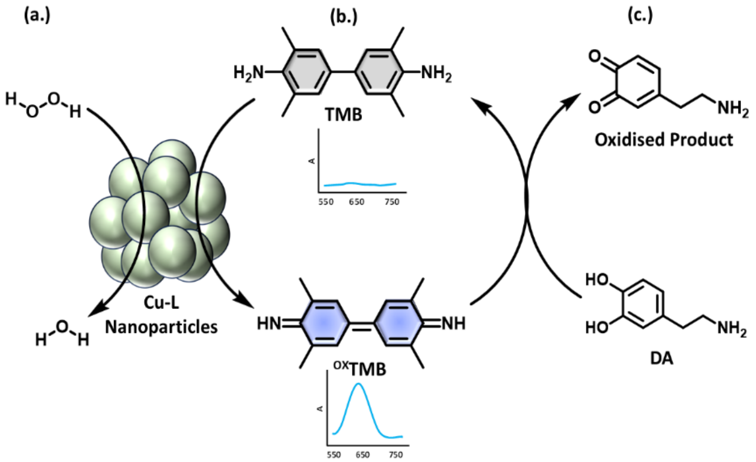

Figure 1. Graphical abstract: (a) POD enzyme-like catalytic activity of Cu-L bionanozyme which is conversion of H_2O_2 into water. (b) Oxidation of TMB during the conversion of H_2O_2 into water, oxidised product is ^{ox}TMB (652nm). (c) Detection of neurotransmitter DA by using the reduction reaction of ^{ox}TMB molecules.

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P-210

Base-Induced Decarboxylative 1,1-Alkoxy Thiolation via Hydrothiolation of Vinylene Carbonate

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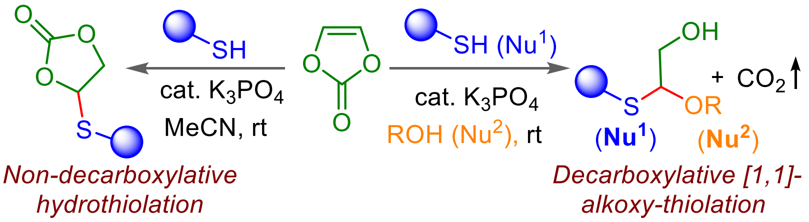
Traditionally the 1,1 or 1,2-functionalization of alkene occurs via the participation of a nucleophile and an electrophile originating from the same reagent. However, the functionalization of alkenes with two nucleophilic partners is scarce. Here, base-mediated 1,1-difunctionalization of vinylene carbonates has been achieved using two different nucleophiles viz. thiol and alcohol. In alcoholic solvents, decarboxylation occurs at room temperature providing a 1,1-difunctionalized product where vinylene carbonate serves as an ethynol (C2) synthon in this three-component reaction. On the other hand, in acetonitrile exclusive hydrothiolation occurs under the basic condition at room temperature. This room-temperature decarboxylation occurs due to the participation of hydrogen bonding interaction between the carbonyl oxygen of vinylene carbonate and the alcoholic –OH group and the non-bonding electrons of sulfur. This reaction is initiated via a radical-mediated pathway which is facilitated by base and oxygen. This methodology features switchable selectivity, broad substrate scope, easy operation, green matrices, and gram-scale synthesis.



- divergent thiolation
- metal-free protocol
- only base as additive
- decarboxylation at rt
- 1,1-difunctionalization
- switchable selectivity

Figure 1

References

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P-211

Sustainable offset ink using Fluorene-Based Schiff base pigment for anti-counterfeiting and latent fingerprint detection

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Counterfeiting of currency, valuable documents, and branded products continues to pose a major challenge for governments, businesses, and consumers globally, resulting in serious financial, safety, and health risks [1]. In the quest for advanced fluorescent pigments, a fluorene-based Schiff base (OAF) was synthesized through a straightforward, one-step, cost-effective process, yielding a bright orange fluorescence. The synthesized molecule was combined with upconverting pigment for enhanced security features and oil-based ink was formulated for offset printing, demonstrating excellent photophysical and rub resistance properties. The ink exhibited orange fluorescence under a 365 nm light source and green emission under a 980 nm source, making it difficult for forgers to replicate. Additionally, latent prints play a crucial role in linking suspects to crime scenes and reconstructing criminal activities [2]. Effective forensic identification heavily depends on the proper visualization and preservation of latent fingerprints [3]. This material proves valuable in forensic science for developing latent fingerprints and it is effective in analysing levels 1, 2, and 3 features.

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P-212

Beyond the Chain: Impact on Charge Transport in a π-stacked Polymer in Organic Electronics

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Conventional electronic technologies have been subject to certain limitations that have become increasingly evident with the downfall of Moore's Law. One major limitation has been the shrinking of discrete devices like transistors, which has been a key driver of performance improvements over the years. However, as the size of transistors approaches atomic levels, it becomes more difficult to reliably manufacture them and prevent leakage of electrical current, leading to decreased performance and increased power consumption. Another limitation is the heat generated by electronic devices, which has become a significant challenge as devices become smaller and more densely packed [1, 2]. These limitations have driven researchers to explore new technologies. The potential of semiconducting polymers/foldamers in electronic applications, such as organic thin film transistors (OTFTs), solar cells, and flexible electronics, has garnered considerable attention. These materials are appealing due to their low-cost processing, flexibility, and unique optoelectronic properties, including high absorption coefficients and low energy bandgaps, biodegradability, and environmental friendliness [3]. The charge transfer properties of organic polymers are heavily influenced by their molecular structure, which has a significant impact on the efficiency of organic electronic devices. Therefore, it is crucial to comprehend and regulate the molecular architecture of these materials to boost device efficiency.

We studied with periodically grafted aromatic polyamides ($P1PEG_{550}$) mimicking higher-order structures like β-sheet with related functions, particularly in charge transport (through space) applications. We conducted a comprehensive analysis of the overall bulk structure of the polymer, with the interaction of guest molecule pyrene ($P1PEG_{550}$:Pyrene) too. In particular, we intend to explore these aromatic polyamides for through-space charge transport (TSCT) applications in the context of their higher-order arrangements. Notably, the incorporation of guest molecules resulted in significant enhancements in the structural coherence of these aromatic polyamides. Such folded structures open an efficient charge transport channel across the ordered π-domains of the host-guest complex. The current density ($\sim 10^{-4}$ A/cm^2) obtained in the vertical charge transport setup was remarkable, considering the transport operates exclusively through-space mechanism. The same material exhibits a less efficient charge transport ($\sim 10^{-10}$ A) in horizontal setup, indicating a preferential alignment of π-domains within the bulk structure. We also found that substrate surface chemistry can impact the orientation of the π-folded domains. Devices fabricated on hydrophilic glass exhibited significantly higher lateral currents ($\sim 10^{-5}$ A) for host-guest complexes than those on unmodified glass substrates, underscoring the potential of these aromatic polyamides for electronic applications through careful substrate selection.

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P-213

Fluorene-Conjugated Naphthalimide: A Novel Fluorescent Probe for H_2S Sensing and Cellular Imaging

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Naphthalimides are widely known for their remarkable fluorescence and electrochemical properties, making them highly suitable for fluorescent dyes, sensors, and organic electronics applications. We designed a novel fluorophore, FLR-NNAP, by attaching 4-nitro naphthalic anhydride to amino-fluorene via imidation.

The molecule was further analyzed for its interaction with carbon monoxide and hydrogen sulfide, focusing on binding energy and HOMO-LUMO energy gaps in both ground and excited states. Results demonstrated an enhanced interaction of FLR-NNAP with hydrogen sulfide compared to carbon monoxide, particularly due to the nitro group's interaction with H_2S.

FLR-NNAP has emerged as a promising cell imaging dye due to its ability to effectively sense endogenous H_2S with impressive fluorescence intensity. Beyond its optical capabilities, FLR-NNAP has also demonstrated its utility as an electrochemical sensor for H_2S detection, broadening its applicability in biological imaging and electrochemical sensing technologies. This multifunctionality positions FLR-NNAP as a versatile tool for advanced research in bioimaging and sensing.

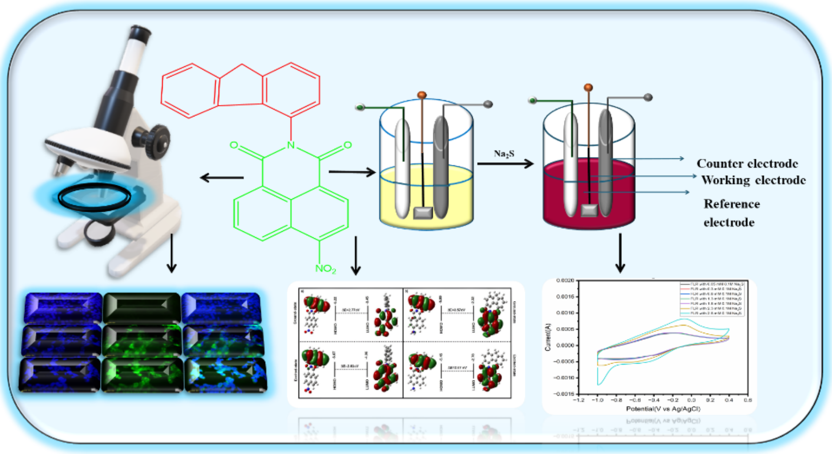

Figure 1. Graphical abstract of FLR-NNAP for bioimaging and electrochemical sensing of Na_2S

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P-214

Efficient Synthesis and Structural Insights of a New Class of Benzo-extended Thia-quasi[7]Circulenes

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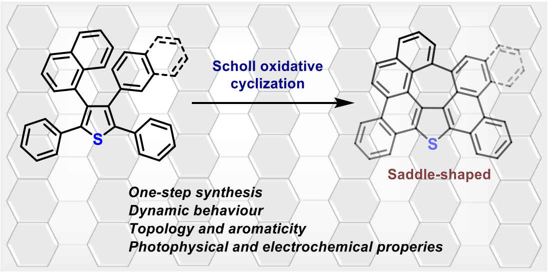
In recent years, hetero[*n*]circulenes, distinguished by their unique topologies and chemistry, have attracted significant attention due to their distinctive geometries and photophysical properties. These polycyclic aromatic molecules have emerged as promising research subjects, particularly in the contexts of their use as templates for 3D nanocarbons, their topology-driven aromaticity, chiroptical properties, and potential material applications. [1-2] While carbon-based quasi[7]circulenes have been reported,[3] the exploration of hetero-quasi[7]circulenes remains relatively underdeveloped. Despite a few existing examples, their synthesis is often hindered by complex procedures and low yields,[4] likely due to the increased strain introduced by integrating heptagonal units into larger polycyclic aromatic hydrocarbons (PAHs). To overcome these challenges and unlock the potential of hetero-quasi[7]circulenes, we have developed a novel synthetic strategy to access benzo-extended thia-quasi[7]circulenes from appropriate precursors. Our approach hinges on designing key precursors amenable to intramolecular oxidative (Scholl) coupling- a powerful technique for constructing heteroatom-embedded quasicirculenes, circulenes, and nanographenes from simple heteroaromatic molecules. [5-8] By employing suitable tetraarylthiophenes, we have successfully achieved the efficient one-step synthesis of thia-quasi[7]circulenes. The intriguing optical and electrochemical properties of these hetero-quasi[7]circulenes underscore their potential applications in various organic electronic devices.



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Synthesis, Characterization, and In-silico studies of Hydrazide-hydrazone linked Coumarin Glycoconjugates

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Keywords: Coumarin, Hydrazide-hydrazone linker, Glycoconjugate, Molecular docking

Abstract: Coumarins, known for their wide range of pharmacological properties, have been extensively studied and utilized in drug discovery and development.[1] Carbohydrates are considered a promising partner for conjugation with heterocycles due to their polyfunctional, water-soluble, and non-toxic nature and the presence of several unique stereochemical and functional characteristics. Therefore, the incorporation of sugars into coumarin scaffolds enhances their solubility, bioavailability, and target specificity, making them attractive candidates for various biomedical applications.[2] Here, we present the synthesis of new hydrazide-hydrazone-linked coumarin glycoconjugates in a multistep reaction protocol that involved the synthesis of coumarin nucleus by Knoevenagel condensation followed by its conversion to coumarin hydrazide and then its coupling with glycosyl ketones. The target compounds were further characterized by spectroscopic methods such as ^{1}H NMR, ^{13}C NMR, FT-IR, and HRMS. The anticancer property of compounds was further studied through molecular docking and molecular dynamics studies.

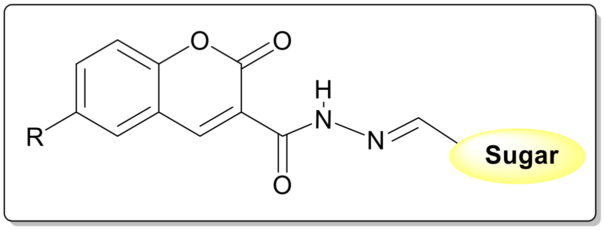

Fig. 1. Representative structure of hydrazide-hydrazone bridged coumarin glycoconjugates

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P-216

All-Liquid Transistor via Topochemically Polymerized chiral Interface Architectures for NO_2 Sensing

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The inherent limitations of conventional solid-state electronics, including their lack of reconfigurability, recyclability, and dependency on non-renewable materials, have catalyzed the development of liquid-based electronic systems. Advanced materials such as liquid metals, conductive polymers, and ionic liquids exhibit dynamic physicochemical properties, offering enhanced flexibility, structural adaptability, and sustainability. Herein, we report the fabrication of an all-liquid chiral transistor via topochemical polymerization at a liquid-liquid interface, a process that generates a structurally jammed, conductive polymeric network. This interfacial polymerization facilitates the formation of a highly ordered, percolating polymeric film that exhibits enhanced charge transport properties due to its unique conjugated backbone. The resulting transistor operates as a p-type semiconductor with exceptional sensitivity, capable of detecting toxic gas like NO2 down to parts-per-billion (ppb) concentrations. Furthermore, this liquid-based transistor demonstrates superior response and recovery kinetics compared to its solid-state counterparts, attributed to the dynamic reconfigurability and enhanced diffusivity at the liquid-liquid interface. The system's surface chemistry and fabrication at ambient conditions underscore its potential as a transformative platform for next-generation, environmentally sustainable gas sensors.

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P-217

Bimetal embedded nitrogen-doped carbon derived from conjugated macrocyclic polymers as electrocatalysts for oxygen reduction reaction

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The synthesis of earth-abundant metal-based electrocatalysts for deploying electrochemical energy devices has become an area of considerable interest. To date, only platinum-based electrocatalysts are known to deliver impressive current because of electrochemical oxygen reduction reactions. However, the factors related to cost and scarcity have aggrandized the research for non-precious metal electrocatalysts. Hence, we focussed on the development of a non-noble metal-based electrocatalyst by using a facile Friedel-Crafts reaction. The synthesized nitrogen-doped bimetallic electrocatalyst possessed abundant structural defects, mesopores, and nitrogen content which are presumed to contribute towards the oxygen-reduction. The obtained electrocatalyst also showed optimum results toward stability and methanol tolerance. Therefore, this work can contribute to the facile synthesis of bimetallic electrocatalysts with non-noble metals to explore their applications in ORR.

P-218

Tetraarylpyrrolo[3,2-b]pyrrole-BODIPY dyad: A Molecular Rotor for FRET based Viscosity Sensing

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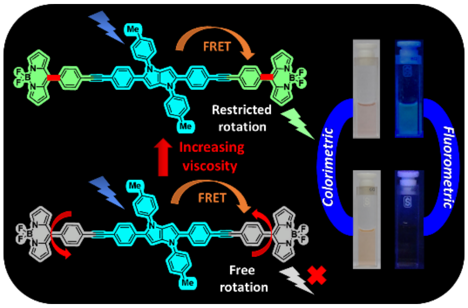

Molecular dyads made up suitably matched optical properties of a donor chromophore (absorbs at lower wavelengths) and an acceptor molecule (absorbs at higher wavelengths) can act as a fluorescence resonance energy transfer (FRET) system.[1] Enhanced pseudo-Stokes shift of these dyads are highly useful for developing chemical sensors as well as advanced bio-imaging agents.[2] With the aim to develop a FRET based viscosity sensor, two dyad molecules, **1** and **2**, comprising of tetraarylpyrrolo[3,2-b]pyrrole (TAPP) (donor) and boron-dipyrromethene (BODIPY) dyes (acceptor) were designed. TAPP is a blue energy donor which is easy to synthesize and functionalize as compared to other well-known blue energy donors like pyrene, perylene etc. This is the first report of using TAPP as an energy donor in BODIPY based dyad molecules. Dyads were synthesized via acid catalysed multicomponent reactions followed by Sonogashira coupling. In both the dyads, BODIPY and TAPP moieties are linked through phenylethynyl linkers. In dyad **1**, substituted BODIPY (fluorescent) was used whereas in dyad **2** is made up of unsubstituted BODIPY (non-fluorescent) dyes which allow free rotation of the BODIPY dyes i.e. dyad **2** can act as molecular rotors. This was supported by X-ray crystallographic and DFT optimized structures. Spectroscopic and electrochemical studies confirmed the presence of both TAPP and BODIPY dyes in dyads with no electronic interactions which is suitable for FRET. In dyad **1**, on excitation at the TAPP moiety, complete quenching of TAPP fluorescence and observation of greenish yellow fluorescence of BODIPY suggests fast energy transfer from TAPP to BODIPY unit (ETE > 99%). Ultrafast fluorescence and transient absorption spectroscopic studies of dyad **1** showed TAPP to BODIPY energy transfer in 480 fs ($k^{ET} = 2.1 \times 10^{12}\ s^{-1}$). This result was rationalized by theoretical Förster formulations.

In case of dyad **2** also fast energy transfer from TAPP to BODIPY unit (ETE > 99%) was observed but due to the non-fluorescent nature of naked BODIPY dyes, no fluorescence emission was observed from BODIPY moiety. Importantly, with increasing solvent viscosities, emission from the BODIPY moieties increases due to restricted rotation of the BODIPY moieties. Plot of logarithms of fluorescent intensity of dyad **2** and viscosity of the solution showed a good linear correlation obeying Förster-Hoffmann equation. Non-fluorescent dyad **2** in methanol became greenish yellow fluorescent in methanol/glycerol (1:1) solvent. Further, with increase in temperature of methanol/glycerol (1:1) system, as the viscosity decreases, the fluorescence also starts decreasing. Thus, the dyad **2** is capable of sensing the viscosity of the medium via FRET based "Off-On" mechanism. This type of viscosity sensor with very large pseudo-Stokes shift and increased sensitivity will be useful for future advancement of chemo-bio sensing and imaging applications.

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P-219

Unveiling the Bioactive Potential of Indian Adzuki Bean (*Vigna angularis*) for Nutritional and Health Benefits

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Nutritional benefits of legumes make them an important part of sustainable diets. They are abundant not only in dietary fibres, proteins, and micronutrients but also in bioactive compounds that can manifest a plethora of biological activities [1]. Adzuki bean (*Vigna angularis*), a legume indigenous to India, has garnered attention for its rich nutritional profile and significant bioactive compounds [2]. Our study explored the nutritional profile and phytochemical composition of Indian adzuki beans, focusing on their role in promoting health and mitigating chronic diseases. Using advanced analytical techniques such as UHPLC-QTOF-MS and GC–MS, we identified a diverse array of bioactive constituents, including flavonoids, phenolic acids, hydrocarbons, fatty acids, and terpenes, known for their antioxidant, anti-inflammatory, and anti-obesity properties. Additionally, our findings highlight the presence of 21 essential macro- and micro-elements, majorly potassium, magnesium, and molybdenum, fatty acids, particularly linoleic acid, which is nutritionally beneficial for human consumption, alongside amino acid profiling that revealed a rich array of essential, non-essential, and non-proteinogenic amino acids [3].

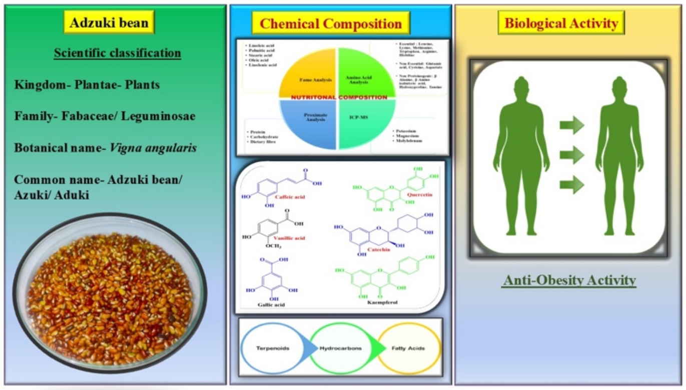

Figure 1. Graphical abstract of bioactive profiling of adzuki bean

The results indicate that adzuki beans not only provide substantial amounts of dietary fiber and protein but also contain potent bioactive metabolites that can enhance metabolic health. These findings emphasize the importance of incorporating adzuki beans into dietary practices, offering a sustainable approach to nutrition while addressing pressing health concerns such as obesity and hyperlipidemia. The adzuki bean thus emerges as a valuable addition to health-promoting foods, warranting further exploration into its applications in preventive healthcare and functional nutrition.

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P-220

Development of a Two-Step Sensitive Fire Alarm System Using Fire Retardant Cotton-Based Materials

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In recent years, the increasing frequency of fire incidents has posed significant threats to human life, the economy, and the environment. To mitigate fire risks, various strategies have been implemented, with a focus on fire-retardant materials and fire alarm systems for early detection and warning, helping to prevent uncontrolled fires and their devastating effects. Traditional fire sensors, however, are often limited by their activation only at certain smoke concentrations, reducing their efficacy in large, open areas.[1] Among commonly used materials, cotton, valued for its renewability and widespread industrial application, is highly flammable with a limiting oxygen index (LOI) of around 18%, making it particularly susceptible to fire-related damage. This has driven efforts to develop halogen-free flame retardants, which are environmentally friendly, non-toxic alternatives to traditional treatments. Recent advances in this area focus on creating effective flame retardants for cotton fabrics, aiming to reduce the risk of ignition and provide greater fire safety in various applications.[2-3]

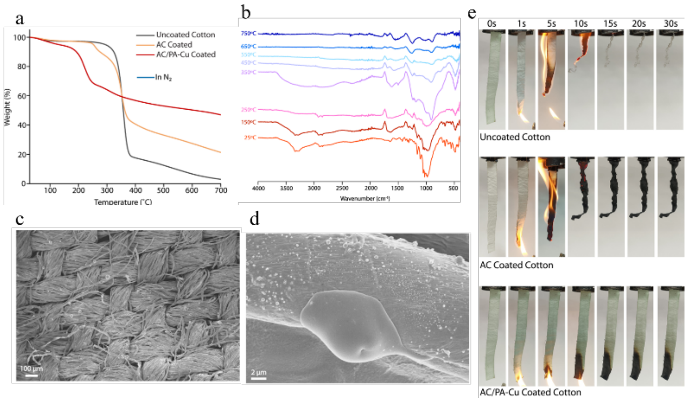

Figure 1. (a) TGA, (b) TG-IR of cotton samples (c-d) FESEM Images showing protective layer formation and (e) Vertical flammability test of AC/PA-Cu coated fire-retardant cotton.

In this study, we designed a fire-retardant coated material which is both biodegradable and economically viable through dip-coating technique. Inspired by the traditional Indian practice of applying mud coatings to houses to protect against heat, cold, and fire hazards. Our coating process involves an initial layer of amino clay (AC) which to the best of our knowledge has not been explored for the application of fire retardancy yet, followed by a secondary layer of phytic acid and copper phosphate complex, which collectively impart enhanced fire resistance to the material. We utilized AC/PA-Cu coated cotton fabrics for device fabrication showing LOI of 61.3 %, which demonstrated exceptional fire retardancy and excellent electrical conductivity. These properties make the material highly suitable for early fire detection applications, enabling its use as a two-step sensitive fire alarm system.

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P-221

Synthesis of Ca-Al Layered Double Hydroxide-alginate beads with potential application as adsorbent for water/wastewater treatment

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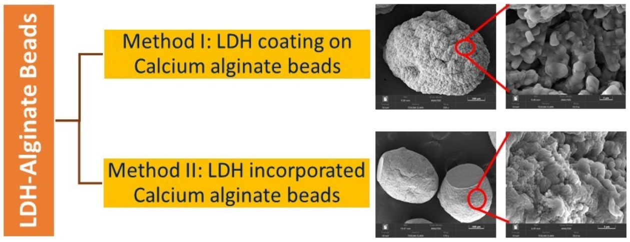
Layered double hydroxides (LDH) are inorganic anionic clay materials possessing a positively charged metal ion layer balanced by interlayer anions. LDHs have been known for the removal of anions and oxyanions through different mechanistic approaches like surface adsorption, interlayer anion exchange, and reformation effect (memory effect). [1] Sodium alginate is a nontoxic and biodegradable natural polymer; when exposed to chelating ions such as calcium, it forms calcium-alginate beads. [1,2] Due to the practical difficulty in the separation process, the powder adsorbents are not employed in wastewater/filtration treatment systems. The bead is one of the most widely used supporting materials to immobilize enzymes, proteins, and other functional materials. The synthesis of these calcium alginate-LDH beads is a simple and cost-effective method, and the Ca-Al LDH is immobilized in the calcium alginate beads through the in-situ synthesis methods. The entrapment of active materials (LDH) in the calcium alginate beads will ease the separation process and enhance the active surface area, leading to increased adsorption capacity. [2]



Scheme: Synthesis methodology and morphology of the LDH-alginate beads.

The objective of the present study was to synthesize LDH-alginate beads by entrapping Ca-Al LDH into calcium alginate beads characterize and apply them as adsorbent for water/wastewater treatment. The LDH-alginate composite beads were synthesized by two different techniques. The first method includes the preparation of the calcium alginate beads followed by coating with LDH by dipping in the LDH dispersion for about 24 hrs, removing from the LDH dispersion, washing with distilled water and air drying. In the second method, pre-synthesized LDH was dispersed in the sodium alginate solution, then the standard method of calcium alginate bead preparation was followed, using a co-extrusion technique, which ensures the homogeneous distribution of LDH within the alginate matrix, enhancing structural stability and adsorption performance. The LDH-alginate beads obtained by the two methods were characterized by FE-SEM, EDS, and XRD to analyze the morphology, chemical composition and crystallographic phase(es). The ionic nature and the functional groups were determined by zeta potential analyzer and FTIR spectrometer.

The present paper describes the physicochemical and morphological properties of the synthesized LDH-alginate beads and the influence of the synthesis method on their physicochemical and morphological properties. The potential application of the LDH-alginate beads and their robust framework as a sustainable solution for water/wastewater treatment will also be discussed.

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P-222

Surface-Modified Tremella Flower Resembling Mixed Metal-oxide Microsphere as Effective Active Materials for Energy Storage

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Strategically modulating the morphological structure of metal oxides has consistently influenced the electrochemical performance of redox reactions in energy storage applications.[1] Hollow and porous microstructures are particularly attractive for energy storage devices, especially supercapacitors, as they enhance their functional properties. Mixed metal oxides, compared to single metal oxides, offer improved electrical conductivity due to their lower activation energy for electron transfer.[2] Their ability to exhibit multiple oxidation states supports rich redox reactions, resulting in higher specific capacitance, while also allowing significant flexibility in structure and morphology.

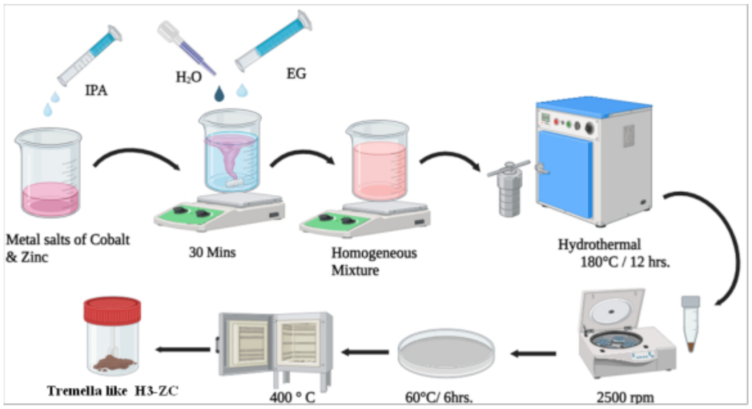

Figure 1. Graphical abstract for the synthetic route for H3-ZC.

The 3D tremella flower-like hierarchical microspheres (Mixed A, B) H3-ZC, along with the ultra-thin hierarchical sheet-like (A) H1-C and hexagonal rod-like (B) H2-Z structures, were effectively synthesized using a hydrothermal technique. The unique hierarchical tremella flower-like microspheres, featuring numerous mesoporous channels, provide a large surface area of 115.210 m^2/g. Additionally, they exhibit synergistic effects from two different metal cations within a single crystal structure. These properties result in high supercapacitor performance, with a specific capacitance of 1232 F/g at a current density of 1 A/g and a capacitance retention of 93% at 5 A/g after 5000 charge-discharge cycles. These findings suggest that H3-ZC is a promising material for energy storage devices.

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P-223

Efficiency enhancement of porous coordination polymers based supercapacitor by implementation of organic redox mediator

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Quest to improve the efficiency of supercapacitors seems to be a perpetual one. The task requires innovation in development of sophisticated electrode and electrolyte materials. Porous coordination polymers (PCPs), also known as metal organic frameworks (MOFs), while serving as an emergent material, have their shortcomings which include low intrinsic conductivity, electrolyte incompatibility and reduced electrochemical stability.[1] These limitations can be obstructive in practical applications, but can be overcome by assorted techniques. These techniques include addition of composite materials to PCPs, optimization of electrolyte, and surface modifications by annealing process.[2] In this presentation, we will elaborate the utilization of our organic redox mediator in improvement of the electrochemical performance of the prepared PCPs and an augmentation in overall efficiency of the supercapacitor.

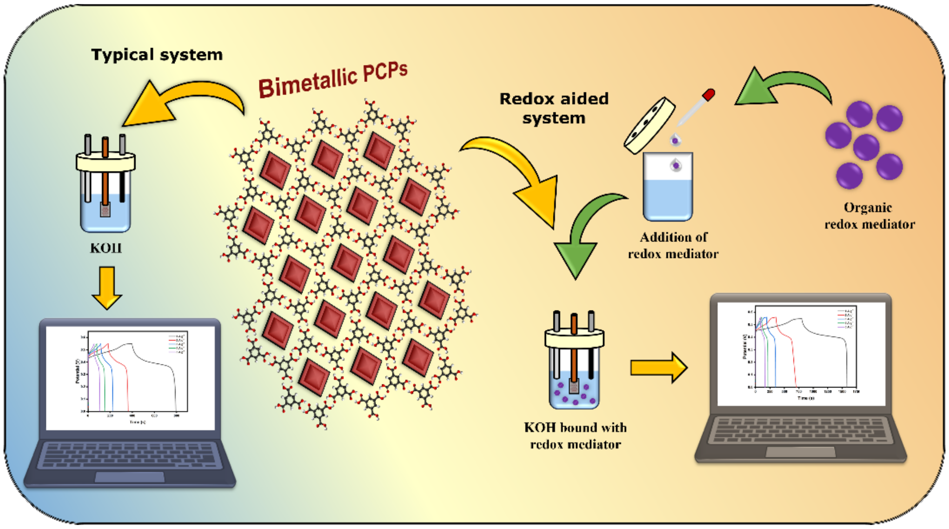

Figure 1. Graphical abstract of the redox aided system for supercapacitor

Herein, a mesoporous bimetallic PCPs were synthesized, having high surface area and are utilised as active electrode material. The prepared material was studied in a half-cell system, where excellent electrochemical properties were observed. A novel redox mediator in organic potassium salt, bound with KOH were implemented to improve the electrochemical performance of the prepared material. This system showed a maximum specific capacitance of 931.47 F g^{-1} at the current density of 1 A g^{-1}. The material retained 88.23% of its original capacitance after 5000 charge-discharge cycles, which was not affected in the presence of redox mediator, indicating that the material was not degraded by augmentation of its performance. This study indicates an improvement in overall efficiency of the material by implementation of the proposed redox mediator in the electrolyte.

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P-224

Construing the interactions of coumarin derivatives with the main protease of stomach pepsin using spectroscopic and computational analyses: insights into the binding thermodynamics, anti-fibrillation studies and enzymatic assay

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Pepsin is often utilized as an important prototype for studying the interaction of small molecules with proteins in the context of digestive proteases [1]. The binding interaction between pepsin and ligands is critical for understanding the molecular process underlying pepsin's function and developing medications that can modulate its activity. Therefore, this study explores the interaction between pepsin and two bioactive compounds umbelliferon (UMB) and 4-methyl-umbelliferone (4-MU) through a combination of multi-spectroscopic and computational techniques. Results from steady-state fluorescence, excited-state fluorescence lifetime, and UV-vis absorption analyses indicated that UMB and 4-MU binding to pepsin followed a static quenching mechanism. Circular-dichroism (CD) and Fourier transform infrared (FT-IR) spectroscopy reveal significant conformational changes in pepsin during ligand binding. Thermodynamics data suggested a positive ΔH and ΔS for both the complexes, indicating hydrophobic forces played a dominant role in the binding process and the negative ΔG value signifies a spontaneous complexation formation. Additionally, one research study indicates that maximum pepsin fibril formation occurs at neutral pH [2]. Investigating amyloid formation at this pH range is crucial, as several diseases associated with amyloid deposits are observed under similar conditions. Remarkably, both UMB and 4-MU exhibit potent inhibitory effect on pepsin fibrillation, as evidenced by Thioflavin T (ThT) and Congo red (CR) binding assays, complemented by fluorescence microscopy and field emission scanning electron microscopy (FESEM) observations. Kinetic analysis reveals an uncompetitive inhibition of pepsin activity by UMB/4-MU. To further elucidate the molecular basis of these interaction, molecular docking and molecular dynamics (MD) simulation offered insight into the binding affinity and flexibility of pepsin upon complexation with UMB and 4-MU [3].

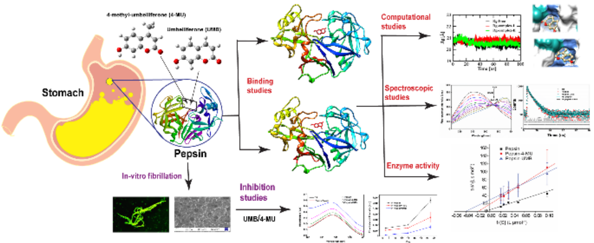

Figure 1. Schematic representation of the binding of bioactive coumarins (UMB/4-MU) with pepsin, along with their inhibitory effects on protein fibrillation and the enzymatic assay measuring pepsin activity in the presence of these ligands.

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P-225

Solute Dynamics of a Hydrophobic Molecule in Menthol-Thymol Based Type-V Deep Eutectic Solvent: Effect of Composition of the Components

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Type V deep eutectic solvents (DESs) are a newly emerging unique class of solvents obtained by physically mixing followed by heating of non-ionic components and these solvents shows large negative deviations from thermodynamic ideality. Compared to Type I-IV DESs, Type V DESs are less explored and their physical chemistry is in their nascent stage[1]. In this work, we have chosen menthol-thymol (MT)-based Type V DES for our working media. Solvent and rotational dynamics were studied using a well-known solvatochromic probe, Coumarin 153 (C-153). We have prepared MT based DESs following the reported procedure at three different molar compositions of menthol(M): thymol(T) (1:1 named as M1T1, 1:1.5 named as M1T1.5, 2:1 named as M2T1) for our study. Time-resolved emission spectra (TRES) were constructed with the variation of temperature and utilizing TRES the decay of solvent correlation function (C(t)) were plotted for each DESs. We have correlated the solvent relaxation time in these DESs as a function of viscosity. The decay of solvent relaxation was found to be bi-exponential (where the slow component shows temperature dependence).

Compared to the iso-viscous choline chloride based DESs, these solvents yield a much higher value of solvation times indicating the presence of nanostructure domains or clusters. Significant viscosity decoupling of the solvation times also suggest the same. Also, the solvent structure outside the first solvation shell varies appreciably with the variation of the components of DESs. The time-resolved anisotropy decays were also collected to perceive the rotational relaxation dynamics of C-153 as a function of temperature. We have analysed the rotational dynamics of C-153 in Type-V DESs employing the Stokes-Einstein-Debye (SED) hydrodynamic model[2]. All the DESs studied demonstrate a good correlation with the SED model with little deviation. The rotational relaxation dynamics were found to be sub-stick at low viscosity (or at high temperatures) for all the molar compositions. Using the Arrhenius-type equations, we have correlated the activation energies for the rotational motion of C-153 with both the viscous flow and non-radiative pathways for all the DESs.

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P-226

An efficient and eco-friendly synthesis of novel nitro functionalized pyrroles and 1,4-dihydrpyridines using DMAP as an efficient catalyst

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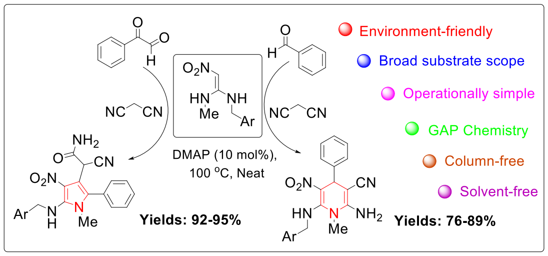

Scheme 1. Graphical abstract for the solvent-free synthesis of nitro pyrroles and 1,4-DHPs

Nitrogen heterocycles such as substituted pyrroles are essential scaffold which present in hemoglobin as well as several natural and synthetic compounds with significant pharmacological properties.[1] Among the functionalized pyrroles, nitropyrrole derivatives are interesting class of compounds that exhibits diverse biological activities [2] and on the other hand 1,4-dihydropyridines and analogues are typically found in natural products and the core scaffolds are present in various medicinally approved drugs.[3] As a consequence, significant attention has been made toward the synthesis of nitro-pyrrole and 1,4-dihydropyridine skeletons.

The development of eco-friendly and efficient synthetic methodologies is crucial for advancing sustainable chemistry.[4] In this work, we present a novel and environmentally benign route for the synthesis of nitro-functionalized pyrroles and 1,4-dihydropyridines using DMAP (4-Dimethylaminopyridine) as a catalyst. We carried out the reaction of nitroketene-N,N-acetal, with aromatic aldehydes and malononitrile for the synthesis of 1,4-dihydropyridines, and similarly pyrrole derivatives also prepared by using arylglyoxal monohydrate instead of aromatic aldehydes with malononitrile and nitroketene-N,N-acetal under solvent-free condition as depicted in the above scheme.

The methodology offers several advantages, including mild reaction conditions, high yields, and the use of less hazardous reagents, aligning with the principles of green chemistry. The use of DMAP, a cost-effective and readily available catalyst, facilitates the reaction efficiently, reducing the environmental footprint. Furthermore, the synthesized compounds exhibit promising potential for applications in pharmaceutical and material science, particularly as intermediates in the development of bioactive molecules. This approach exemplifies a significant step toward the development of sustainable and scalable processes in organic synthesis.

Key words: Arylglyoxal monohydrate, DMAP, 1,4-Dihydropyridines, Pyrroles, Solvent-free, nitroketene-N,N-acetal

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P-227

Nanostructural Characteristics and Oxidative Reactivity of Diffusion Flame Generated Soot using Methyl Crotonate and Methyl Butyrate as Surrogate Fuels

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Soot emissions from combustion engines pose significant risks to both the environment and human health, making it crucial to understand soot formation and explore mitigation strategies, particularly through the use of biodiesel additives. This study focused on the enhanced oxidative reactivity of soot and how it is influenced by the nanostructural properties of soot produced from distinct blends of saturated and unsaturated biodiesel surrogates, specifically, methyl butyrate (MB) and methyl crotonate (MC)—with diesel. A blend of 25% MB with 75% diesel resulted in the lowest tendency to produce soot and the lowest activation energy for soot oxidation (155.4 ± 2 kJ/mol), in comparison to pure diesel, which exhibited an activation energy of 175.1 ± 2 kJ/mol. The soot was gathered using a smoke point apparatus with a wick-fed laminar diffusion flame under atmospheric pressure.[1]

Detailed nanostructural analysis of the soot was carried out using various techniques, including HRTEM, Powder XRD, CHNS and EDX elemental analysis, BET surface area analysis, Raman spectroscopy, and thermogravimetric analysis.[2] Results showed that MB addition improved combustion efficiency, reduced primary soot particle size, increased interlayer spacing, and enhanced fringe tortuosity, leading to greater crystal disorder and improved reactivity with oxygen. In contrast, the 25% MC-75% diesel blend showed higher soot production and a higher activation energy for oxidation (165.0 ± 2 kJ/mol), likely due to the formation of resonance-stabilized radicals (RSRs), which affected the combustion process.[3] The study effectively demonstrates how structural differences in soot can influence both its formation and oxidation behaviour. These structural impacts are important considerations for developing global kinetic models for biodiesel-diesel combustion systems.

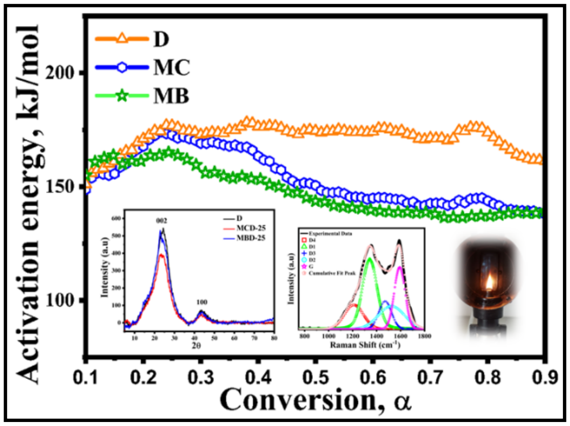

Figure 1. Graphical abstract of nanostructural characteristics and oxidative reactivity of methyl butyrate and methyl crotonate as surrogate fuels.

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P-228

MnO_2 Nanorods on Mesoporous Carbon as a Bifunctional Electrocatalyst for Hydrazine Oxidation and Oxygen Reduction Reactions in Alkaline Media

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Hydrogen production through water splitting plays a crucial role in harnessing zero-carbon green energy. The hydrazine oxidation reaction (HzOR) is considered a viable alternative to the sluggish anodic oxygen evolution reaction. However, HzOR faces challenges due to its high operational potential compared to its low theoretical value, necessitating the use of costly precious metal-based electrocatalysts to reduce overpotential.[1] Additionally, noble metal (Pt)-based catalysts experience slow kinetics for the cathodic oxygen reduction reaction (ORR) and are economically unviable, also suffering from the methanol crossover effect. Therefore, there is a pressing need for cost-effective, non-precious metal-based bifunctional electrocatalysts that can efficiently catalyze both HzOR and ORR.[2] In this context, we developed a straightforward method to create manganese oxide nanorods incorporated into mesoporous carbon (CKT) as a bifunctional electrocatalyst to enhance anodic HzOR and cathodic ORR in alkaline conditions. The synthesized MnO_2/CKT nanocomposite exhibits impressive performance for HzOR, with a low onset potential of 0.7 V vs RHE and a current density of 10 mA cm^{-2} at 0.88 V vs RHE. It also features a Tafel slope of 105 mV $decade^{-1}$ and achieves a maximum current density of 25.6 mA cm^{-2} at 1.4 V vs RHE with 50 mM hydrazine hydrate in 1 M KOH. Furthermore, the MnO_2/CKT catalyst efficiently reduces molecular oxygen, matching the performance of the leading Pt/C catalyst through a 4-electron pathway, with an improved onset potential of 0.95 V vs RHE and a current density of −4.5 mA cm^{-2} in O_2-saturated 0.1 M KOH.

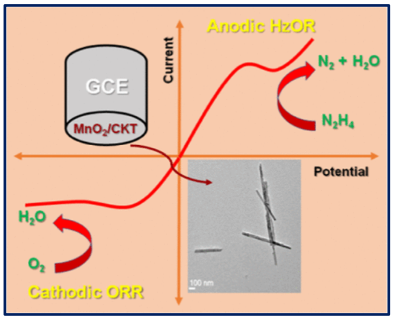

Figure 1. Graphical abstract representing Cathodic ORR and Anodic HzOR using MnO_2/CKT electrocatalyst

Electrochemical impedance spectroscopy and chronoamperometric (i−t) measurements demonstrate rapid electron transfer and high stability at the interface.[3] The exceptional bifunctional electrocatalytic performance of the MnO_2/CKT nanocomposite stems from the synergistic physicochemical properties of MnO_2 and CKT, which facilitate effective analyte diffusion, low charge transfer resistance, and a high density of active sites for catalytic reactions.

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Fabrication of a pH-responsive Moisture-sensitive Actuator for Humidity Detection

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Biomimetic soft actuators[1] are artificial devices designed to mimic the flexible and adaptable movements found in biological organisms. These soft actuators can respond to various external stimuli such as light, temperature, moisture[2], pH, magnetism, and electricity, and can undergo controlled deformation under the stimulation of environmental energy[3]. Their ability to generate complex, natural movements while maintaining a high degree of flexibility and adaptability makes them a promising technology in a wide range of applications such as soft robots[4], microdevices, wearable electronics, biomedical engineering, and sensors. Inspired by this, here, we have reported a three-component bilayered moisture-sensitive actuator mainly consisting of branched polyethylenimine (BPEI), polyethylene glycol diacrylate (PEGDA) and octadecyl acrylate (ODA). Achieved by a casting evaporation strategy, this actuator is formed due to the co-existence of various physical and chemical cross-linking between the components. Due to the balance between the hydrophilicity and hydrophobicity between the two layers, the actuator showed unidirectional bending upon exposure to moisture from all directions. Detailed studies on the effect of pH and the effect of humidity gradient on the behavior of the actuator have also been described. Furthermore, in a more practical approach, the moisture-sensitive actuator was implemented in sensing the humidity of the environment.

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P-230

Elucidation of inhibitory effects of bioactive anthraquinones towards formation of DNA advanced glycation end products (DNA-AGEs)

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DNA, or deoxyribonucleic acid, is the genetic material of living organisms. It carries the genetic information necessary for biological functions, such as directing transcription and translation and aiding in synthesizing RNA, proteins, and enzymes [1]. Prolonged elevations in blood glucose levels lead to non-enzymatic DNA glycation, which generates DNA-AGEs and free radicals that cause structural perturbations in DNA, including strand breaks, depurination, and mutations involving deletions, insertions, and transpositions. These disorders can cause a range of health issues, including complications related to diabetes, neurodegenerative diseases, and age-related conditions [2]. This study focuses on the *in vitro* glycation of calf thymus DNA (ct-DNA) and its inhibition by two anthraquinone derivatives, aloin and purpurin [3]. The formation of DNA-AGEs was characterized using UV-vis and fluorescence spectroscopic methods. The glycation-induced structural DNA damage was observed using circular dichroism (CD) spectroscopy. The analysis of the inhibition of the glycation process by aloin and purpurin was observed by changes in AGEs fluorescence intensity and melting temperature (T_m) of ct-DNA, as well as the presence of a band in gel electrophoresis. Our findings shed light on the inhibitory actions of aloin and purpurin on DNA glycation, suggesting their possible applications in mitigating the adverse consequences linked to increased ribose concentrations. Gaining knowledge of the underlying mechanisms and the potential of these bioactive molecules to inhibit DNA glycation can be very helpful in the development of therapeutic agents that specifically target glycation-related processes.

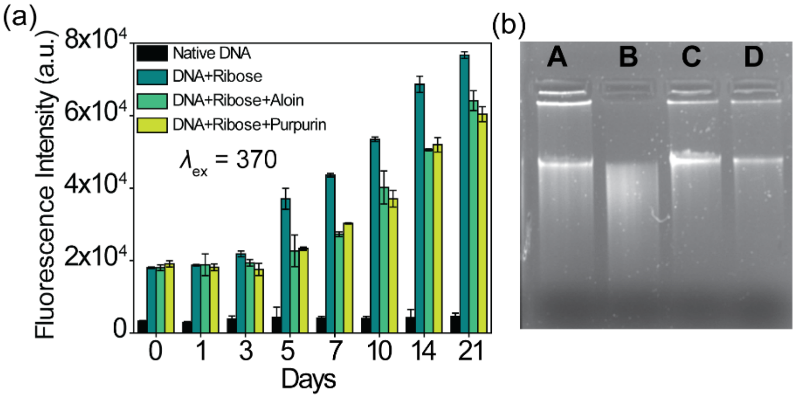

Figure 1. (a) Bar diagram of AGEs fluorescence of native DNA, glycated DNA, and glycated DNA treated with aloin/purpurin (b) Agarose gel electrophoresis of native and glycated DNA. Lane A, B, C and D represent native DNA, glycated DNA, glycated DNA treated with purpurin and aloin.

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P-231

QbD driven extraction, isolation and purification of piceatannol from passion fruit seeds and its cubosomes development, characterization and neuronal cellular analysis

Sandeep Jat

Background: Passion fruit is well utilized for juice and other edible purposes. Passion fruit also contain the seeds and no utilization after juice and other preparation. Passion fruit seed is not explored for its active ingredient isolation and in depth characterization so far.

Purpose: Therefore, it was hypothesized to isolate pure of piceatannol from passion fruit seed using quality by design approach. piceatannol was characterized using NMR, HRMS, SEM, TEM, FTIR and UV.

Study design: According to the framed objectives, the present study reported the complete characterization of markers extracted from PF seed extract, their formulation development and characterization, and the cell line study of PIC-CBs with the additional advantage of being biocompatible.

Methods: Purity assemesent was done using HPLC-DAD. The percent mass yield of 20% and the percent PIC yield of 0.4% were obtained by QbD and provided optimum values of factors that significantly affect the results. It was found to be piceatannol exit in trans from as j values exit between 12-18Hz in NMR data analysis. In addition, purified marker (PIC) encapsulation was carried out to ameliorate its bioavailability, and cubosomes (CBs) were developed to entrap hydrophobic PIC.

Results: The particle size obtained was 96.25 ± 5.23 nm with a zeta potential of -19.3 ± 2.21 mV. SEM micrographs depicted the spherical morphology of PIC-CBs, with an average size of 300-450nm. The characterization from DSC, XRD, and FT-IR reported that the PIC was successfully entrapped in the matrix of CBs, and no interaction was found between the drug and excipients. Moreover, PIC exhibited biphasic release, where 67% of release occurred in 2 hours and provided the sustained release of 90% up to 24 hours. Also, the hemocompatibility and safety of CBs were proved through a hemolysis study (<10% hemolysis). The cytocompatibility was performed using an MTT assay on PC12 cells, and cell adhesion and proliferation studies were carried out with different formulations for a week; therefore, it showed neuronal cell growth.

Conclusion: Therefore, this study concluded that the purified PIC and synthesized formulation can be further used to evaluate the ability of in vivo targeting in Alzheimer’s disease.

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Development of Phosphate Modified Inorganic Layered Double Hydroxide Based Eco-friendly Flame-retardant for Leather

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Flame retardant chemicals are incorporated in or coated on materials to meet the fire safety standards of high-end consumer products. The flame-retardant chemicals for leather available in markets are primarily halogen-based, sulphonated compounds, antimony oxide-based, boron-based and organic phosphate-based compounds. [1] However, most of them are in the SVHC list of REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals*)* as they turned out to be a high-risk threat to ecological and environmental sustainability. [2]

So, the present research work aims to develop a non-toxic, eco-friendly flame retardant for leather application. In order to meet the above objective, an inorganic composite flame-retardant has been designed by combining ammonium polyphosphate (APP) and Mg/Al layered double hydroxide (LDH). [3] The composite flame retardant is expected to function through endothermic de-hydroxylation of the -OH and H_2O molecules in the LDH and enhanced char formation due to the polyphosphoric acid generation from the APP. A series of APP-modified Mg/Al LDH (MAPP) was synthesized by varying APP concentrations between 1-15%. The endothermic enthalpy change (-ΔH) of the synthesized MAPP samples was studied by differential scanning calorimetry (DSC) to understand the heat-absorbing capacity of the chemical to act as a flame retardant. The ionic nature and the hydrodynamic diameter of the samples were analysed as they are essential parameters for leather application. The synthesised composites were characterized for chemical composition, inorganic phase, and functional groups using SEM-EDX, XRD and FTIR. The thermal characteristics [total endothermic enthalpy (ΔH)] acquired from the DSC studies of all the MAPP samples revealed that they have very high -ΔH between 100 to 200 °C, indicating the higher heat absorption capacity of the APP/LDH composite system, thus marking it a potential flame retardant. The developed MAPP was incorporated into leather through the post-tanning operation by following a conventional leather processing technique. The detailed physicochemical characterization of the MAPP samples and the flame retardancy of the MAPP-treated leathers are discussed and compared to the existing commercial flame retardants.

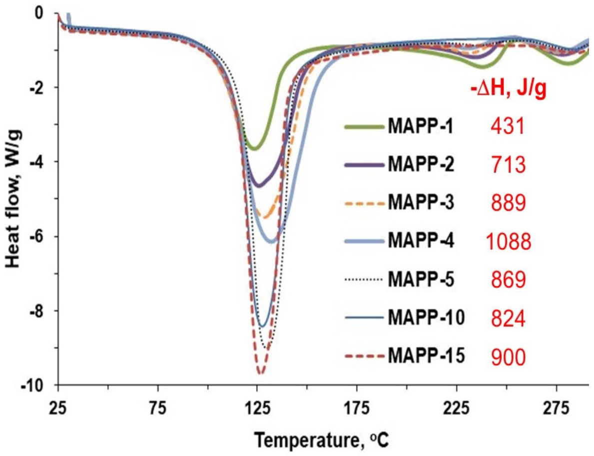

Figure 1. DSC thermograms of the synthesized APP-modified Mg/Al LDH with varying APP concentrations.

MAPP	-ΔH J/g	Zeta Potential mV	Hydro-dynamic d, nm
MAPP-1	**431**	**-7.2**	**1624**
MAPP-2	**713**	**-11.5**	**1557**
MAPP-3	**889**	**-9.2**	**1344**
MAPP-4	**1088**	**-11.2**	**1564**
MAPP-5	**869**	**-14.8**	**1551**
MAPP-10	**824**	**-15.3**	**1837**
MAPP-15	**900**	**-16.7**	**1511**

Table 1. The endothermic enthalpy change, zeta potential and hydrodynamic diameter of the synthesized APP-modified Mg/Al LDH samples.

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P-233

Fe(III)-incorporated porphyrin-based porous organic polymer as a peroxidase mimic for the sensitive detection of glucose and H_2O_2

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Nanozymes i.e., nanomaterials having intrinsic enzyme-like behaviour have flourished over the past few decades due to to their advantages of enhanced stability and effortless storage.[1] Such artificial enzymes can be a perfect alternative to naturally occurring enzymes, which have disadvantages of high cost and limited functionality.[2] Nanozymes typically exhibit greater thermal and chemical stability compared to natural enzymes, making them suitable for use even in harsh conditions.[3] In this work, we report a synthesis of Fe(III)-incorporated porphyrin based porous organic polymer as a nanozyme for the efficient detection of glucose through its intrinsic peroxidase activity and the amperometric detection of hydrogen peroxide. The as-synthesized materials were characterized by solid-state ^{13}C CP-MAS, thermogravimetric analysis (TGA), Fourier transform infrared (FT-IR) spectroscopy, X-ray photoelectron spectroscopy (XPS), powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The porous property of the materials was characterized by N_2 adsorption/desorption isotherms at 77 K.

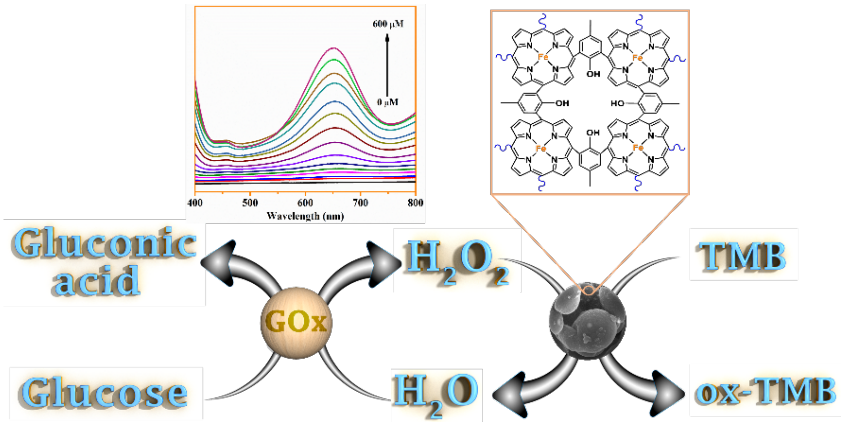

Figure 1. Schematic Representation of peroxidase-mimicking activity of Fe-DMP-POR

The iron-incorporated porphyrin-based conjugated organic polymer (Fe-DMP-POR) owns a spherical morphology with an excellent chemical and thermal stability. Utilizing the peroxidase mimicking activity of the material for glucose detection, a detection limit of 4.84µM is attained with a linear range of 0-0.15 mM. A reasonable recovery range for detection of human blood glucose is also exhibited by Fe-DMP-POR. The as-synthesized material can also perform as a H_2O_2 sensor possessing a sensitivity of 947.67 $\mu Acm^{-2}mM^{-1}$ and a limit of detection of 3.16 µM.

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P-234

Dual C(sp^3)–H and C(sp^2)–H Activation of 8-Methylquinoline *N*-Oxides: A Route to Access C7–H Bond

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The C8-H bond functionalization of heteroaromatic scaffold quinoline has gained a significant progress owing to its various applications in drug discovery, synthetic and material sciences.[1] Recent progress has been made on the functionalization of the C2−H and C8−H bonds of quinoline, whereas studies toward the activation of C5-7−H bonds are scarce, which is due to lower electrophilicity and geometrical inaccessibility for the directing group (DG) on the ring nitrogen to these C−H bonds.[2] On a contrary, quinoline functionalization with a less reactive C(sp^3)−H bond has attracted much attention to construct diverse quinoline scaffolds of interest.[3] Our goal is to merge C(sp^3)−H and C7−H functionalization of quinoline in the relay C−H activation approach for the rapid synthesis of polycyclic structural frameworks.

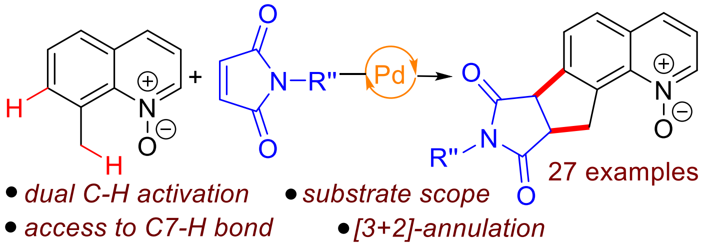

Figure 1. Dual C(sp^3)–H/C7(sp^2)–H activation and annulation of 8-methylquinoline *N*-oxides

Herein, we wish to report the 2-fold activation of C(sp^3)−H and C7−H bonds of 8-methylquinoline *N*-oxides using maleimide as the relaying coupling partner to furnish tetracyclic scaffolds (Figure 1).[4] Maleimides are versatile coupling partners for C−H functionalization/annulation with widespread applications in pharmaceutical and medicinal sciences.[5] The reaction sequence relies on utilizing *N*-oxide as a weak chelating DG, whereas the strong chelating DG yielded the Heck product *via* β-hydride elimination or alkylation *via* [C(sp^3)−Pd] protonation. The 2-fold activation of 8-methyl C(sp^3)−H and C7(sp^2)−H bonds, [3 + 2]-annulation, substrate scope and functional group diversity are the important practical features.

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P-235

Deciphering the Influence of Zwitterionic Surfactants on Pluronic Co-assemblies: A Synergistic Odyssey through Spectroscopic, Microscopic, and Scattering Techniques

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Fundamental investigations into the physical behaviours of pluronic-surfactant mixed assemblies are essential to advance our understanding of molecular interactions at the nanoscale, setting the stage for innovative solutions in drug delivery, diagnostics and other applications of pluronic-surfactant assemblies. While numerous studies have explored the interaction between pluronics and charged surfactants, the realm of research focusing on the integration of pluronics with zwitterionic surfactants—compounds characterized by their simultaneous possession of positive and negative charges—remains scarce. This investigation explores the intricate photophysics of pluronic-zwitterionic surfactant mixed assemblies, utilizing the twisted intramolecular charge transfer (TICT) active styryl dye, trans-2-[(4-dimethylamino) styryl] benzothiazole, as a probe to discern the effects of polarity changes within the assembly microenvironment [1]. By comparing the behaviours of two distinct pluronics at concentrations of 5wt% and 10wt%, F108 and F127 each, which differ in their polyethylene oxide (PEO) and polypropylene oxide (PPO) unit composition, this study systematically examines the impact of zwitterionic surfactants, SB3-12 [Dodecyl dimethyl(3-sulfopropyl) ammonium hydroxide inner salt] and SB3-14 [3-(Myristyldimethylammonio) propanesulfonate]. Through a comprehensive set of spectroscopic techniques, including UV-visible absorption, steady-state emission, time-resolved fluorescence emission studies, significant alterations in the emission spectra and quantum yield were observed upon zwitterionic surfactant addition with multi-exponential emission decay. These modifications suggest a dynamic equilibrium of dye molecules transitioning between various microenvironments within the assemblies, highlighting the interplay between surfactant concentration and the physicochemical properties of pluronic-surfactant systems. Additionally, dynamic light scattering (DLS), Zeta Potential, FESEM, SANS, NOESY, Cryo-TEM and fluorescence lifetime imaging microscopic (FLIM) analyses shed light on the altered hydrodynamic size, charge defining interaction, and in-situ shapes, of the assembly respectively, revealing the substantial impact of surfactant incorporation on the structural and photophysical properties of the assemblies. This research underscores the potential of zwitterionic surfactants to modulate the microenvironmental properties of pluronic-based systems, offering promising avenues for enhancing the applications of such assemblies.

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P-236

Design and Synthesis of Novel Heterogeneous Catalyst for the Carbonylation of Glycerol-to-Glycerol Carbonate with Urea

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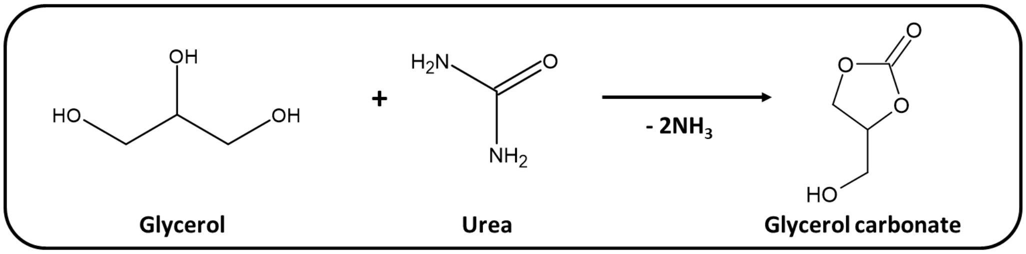
Increasing energy demands and environmental pollution are the two major crises, facing the world today[1]. Alternative energy sources, including biodiesel, play a vital role in reducing our dependency on fossil fuels thereby reducing the major environmental threats[2]. However, biodiesel transesterification has led to surplus glycerol production as a by-product, reducing its market competitiveness. Carbonylation of glycerol to useful chemicals such as glycerol carbonate (GC) is gaining immense importance[3]. Moreover, using urea as a carbonylating agent is an eco-friendly and cost-effective pathway to convert glycerol to GC, as it is also an indirect way to incorporate the greenhouse gas of CO_2 into useful products[2].



Scheme 1. Carbonylation of glycerol with urea to glycerol carbonate (GC)

In this work, we have adopted an innovative methodology to design and synthesize Cobalt-based catalysts and investigated their catalytic activity for the carbonylation of glycerol to GC using urea, for the first time. The prepared catalysts showed excellent yields and selectivity towards GC. The catalysts were thoroughly characterized using various analytical techniques of IR, Raman, XRD, BET, TPD, SEM-EDX, TEM, and XPS analysis, and their physicochemical properties were correlated with their catalytic performance. FT-IR and GC-MS techniques investigated the product formation and the working mechanism. Kinetic studies were also carried out to calculate activation energy. Finally, this study aimed to fabricate a simple, inexpensive, and efficient catalyst for the carbonylation of glycerol to the commercially important product of GC.

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P-237

Room temperature columnar self-assembley of luminescent perylene based molecules with cyanovinylene chromophore

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There is significant demand for molecular functional materials with tailored light-emissive and charge transport properties for their utilization in organic optoelectronic devices. Motivated by such promising properties, we present the synthetic design and emissive and semiconducting properties of aggregationinduced emission (AIE)-active columnar discotic liquid crystals based on cyanostilbene-modified perylene derivatives. Columnar phases formed by the stacking of disc-like molecules with an intimate π-π overlap forms a one-dimensional pathway for the anisotropic charge migration along the columns.[1] Modification of the perylene core resulted in tuning of the photo-physical properties and self-assembly behavior.[2] Here we are going to discuss our efforts with perylene molecule towards opto-electronic applications.

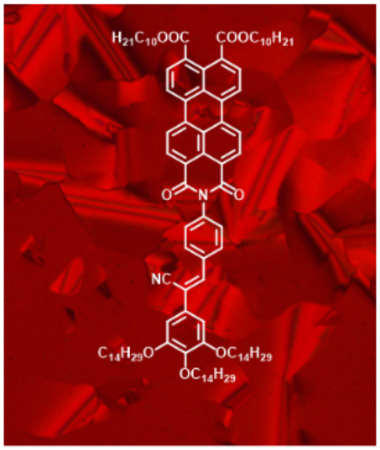

Figure 1. Graphical image of target molecule

Firstly, we have successfully added AIE active cyanostilbene chromophore into perylene which is known to show significant luminescent behavior even after aggregation. The cyanostilbene core was attached with peripheral flexible chains to induce liquid crystalline behavior as well.[3] These room temperature LC because of its high luminescent nature can be utilized in the fabrication of organic light emitting diodes. We have also prepared perylene bisimides with cyanostilbene moiety at both ends which will be highly useful for organic field effect transistors.

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P-238

Aromaticity of Polycyclic Conjugated Hydrocarbons in the Excited States – A Quantum Mechanical Approach

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Polycyclic conjugated hydrocarbons (PCHs) are considered as novel molecules for applications in organic electronic devices due to their unique electronic and self-assembling properties [1]. Here in this work, we have designed a PCH namely biHexadehydro[12]annulene (biHDA) containing three fused antiaromatic units of one cyclobutadiene (CBD) and two Hexadehyro[12]annulenes (HDA). Theoretical studies on the local and global aromatic and antiaromatic properties of biHDA have been performed in its ground states (S_0) and the excited states (S_1, T_1, Q_1) employing Density Functional Theory. To distinguish the aromatic or antiaromatic characteristic of the molecule in its different spin states, the Nuclear Independent Chemical Shift (NICS) value and harmonic Oscillator Model of Aromaticity (HOMA) have been done at GIAO-B3LYP/6-311+G(d,p) level of theory [2].

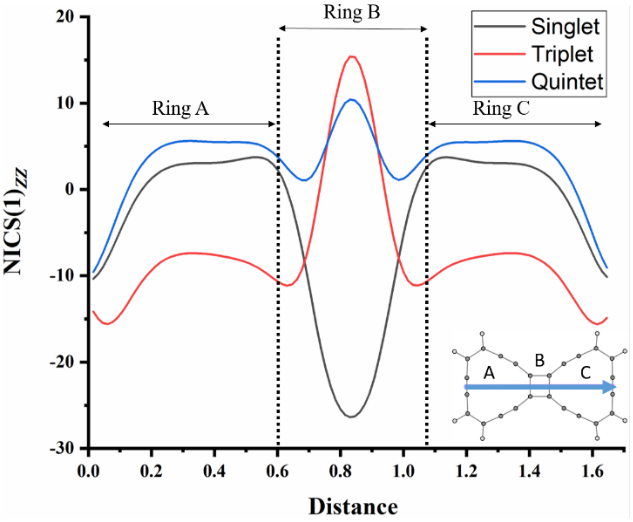

Figure 1. NICS-XY scan of the biHDA in its different spin states employing the GIAO method at B3LYP/6-311+G(d,p) level of theory.

The individual CBD and HDA molecules sustain paratropic ring currents, suggesting both molecules are antiaromatic in nature. However, in the fused biHDA molecule, while the HDA moieties remain antiaromatic, the central CBD ring possesses a strong aromatic character in the ground state (S_0) (Figure 1). Interestingly, in the triplet excited state (T_1), all three rings in the biHDA molecule become antiaromatic, violating Baird's aromaticity rule. However, in the quintet excited state (Q_1), both the HDA rings and the central CBD ring convert to aromatic and antiaromatic in nature, respectively. The anisotropy of the induced current density (AICD) has been calculated to ascertain the above observation. The optical absorption spectra have also been calculated using time-dependent DFT (TD-DFT) calculations, and a strong optical absorption in the visible region (~ 459.31 nm) has been observed. The narrow energy gap between the Frontier Molecular Orbitals ($\square E_{\text{(HOMO-LUMO)}} = 2.05\ eV$) suggests a possible reversible electron transfer property that can be used for potential optoelectronic applications.

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P-239

Caesium Carbonate-Promoted Reaction of Nitro-Substituted Donor-Acceptor Cyclopropanes with Primary Aromatic Amines in Water: Access to β-Enamine Malonates

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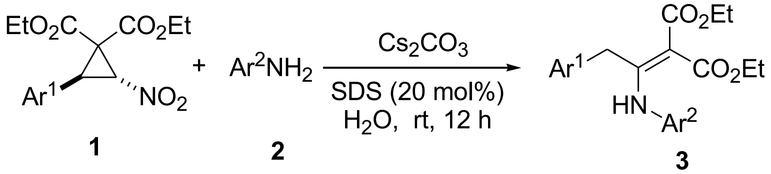
The enamines and their derivatives are versatile synthetic intermediates and are usually synthesized by the condensation of amines with carbonyl compounds, cross coupling reaction between amines and vinyl halides or triflates.[1] Although, a handful of methods are available for the synthesis of enamino esters such as β-enamino malonates, DACs have been rarely used as starting materials for their synthesis.[2] Donor-Acceptor cyclopropanes, especially those containing nitro substituents, have become extremely useful and distinctive building blocks in organic synthesis. [3] As part of our ongoing investigation on exploring the synthetic potential of nitro-substituted donor-acceptor cyclopropanes, [4] we noticed that ring opening/aza Michael addition reaction between DACs **1** and primary aromatic amines **2** in the presence of caesium carbonate and 20 mol% of sodium dodecylsulphate (SDS) in water resulted in the production of β-enamino malonates **3** in good yields (**Scheme 1)**. In the poster, we will discuss the substrate scope and the mechanism of the transformation in detail.



Scheme 1

References:

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P-240

2D NiO/g-C_3N_4 nanocomposite for Photoelectrochemical Water-Splitting for Oxygen evolution Production

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Photoelectrochemical (PEC) water splitting offers a sparkling and sustainable strategy for hydrogen generation, and significant research for enhancing the conversion efficiency of electrocatalysts is underway. Photo Electrochemical (PEC) hydrogen generation is considered as the simplest, economical, clean and efficient way for hydrogen production. Two dimensional (2D) nanocomposite in combination with other 2D material play a vital role for photoelectrochemical splitting of water. In this work NiO/g-C_3N_4 nanocomposite was prepared by varing the amount of NiO in g-C_3N_4. The higher electrochemical and PEC water splitting activity of 2D/2D interface may be due to the more intimate contact between 2D sheets of NiO with g-C_3N_4. Moreover, the effect of NiO loading in nanoheterostructures have been studied towards overall water splitting by varying the ratio of precursors for NiO to that of g-C_3N_4. A A maximum photocurrent density of 20 mA cm^{-2} at an overpotential of 190 mV was observed for oxygen evolution reaction.

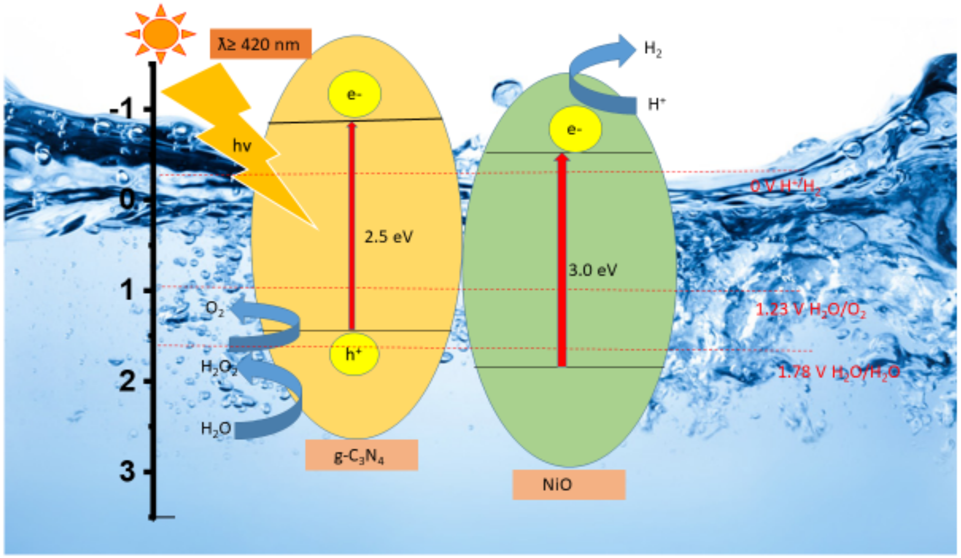

Fig-1. Graphical Abstract of NiO@g-C_3N_4

P-241

ACO/Ag/MFO n-n Heterostructure for Photocatalytic Applications

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Water quality is greatly impacted by the chemical dyes utilized in the textile manufacturing sector. Because they don't cling firmly to the fabric, textile colors leak into aquatic ecosystems as effluent. [1] This means that the ecology and public health suffer greatly when effluent from several textile entities is continuously released into the environment without first being treated. Textile dyes can be harmful to aquatic creatures and contaminate aquatic ecosystems. They also have a risk of entering the food web. [2] The most widely used synthetic dye in the textile industry is methylene blue (MB), which is used in combination with a wide range of other dyes such as rhodamine, methyl orange, congo red, malachite green, and crystal violet. While several environmental remediation techniques are in use, semiconductor-based visible light-responsive photocatalysis has garnered attention globally. Since it uses endless renewable solar energy and produces less hazardous byproducts during photocatalytic degradation, it is considered as the most advantageous technique. [3]

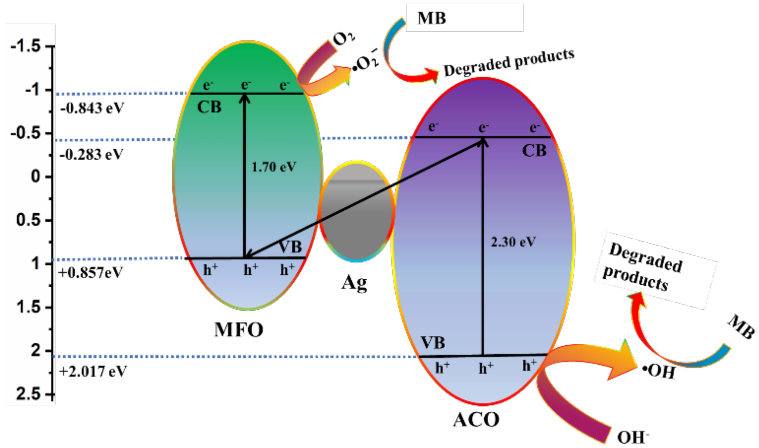

Figure 1. Mechanism of n-n type heterostructure.

Motivated by the previous findings, we have created a nanocomposite known as the ACO/Ag/MFO n-n heterostructure that efficiently breaks down MB in an aqueous solution within a short span of 60 minutes (where ACO & MFO is assigned as Ag_2CO_3 & MOF derived α-Fe_2O_3). The physicochemical properties of the ACO/Ag/MFO heterojunction have also been examined and verified through photoelectrochemical (PECH) studies, SEM, XRD, TEM, XPS, and BET analysis. This study could lead to new avenues for investigating how n-n heterostructure develops as a photocatalyst for the degradation of harmful pollutants, and for investigating its potent real-world applications.

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P-242

Membrane-active amphiphilic EGCG derivatives and their silver nanoformulations as broad-spectrum antibacterial agents

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Bacterial infections are the second leading cause for global mortality and antimicrobial resistance in particular has emerged as a severe threat. Natural products have traditionally been a great source for new therapeutics including various approved antibiotics. In this study, we have strategically modified a natural polyphenol, epigallocatechin gallate (EGCG), into an amphiphilic molecule that can surpass its limitations and transform it into a potent antibacterial agent. Seven EGCG derivatives have been designed, synthesized and assessed for their antibacterial efficacy and mode of action. Among these, **4″-C_{14} EGCG** and **4″-C_{16} EGCG** were identified as most effective antibacterial compounds exhibiting >99% inhibition against *Escherichia coli* and *Bacillus subtilis* at a concentration of as low as 1 µg/mL. They were able to induce intracellular ROS generation and disrupt the integrity of the cell membrane. Further, an enhanced water solubility and antibacterial activity were achieved by synthesizing silver nanoparticles (AgNPs) of the lead compounds. The AgNPs were characterized by UV-Vis, FT-IR, TEM and DLS. The modified AgNPs exhibited a large reduction (16-fold) in the minimum inhibitory concentration (MIC) with significantly improved water-solubility. Notably, it could eliminate drug-resistant strains such as methicillin-resistant *Staphylococcus aureus* (>99% at 100 µg/mL), *Acinetobacter baumannii* (>99% at 10 µg/mL) and *Pseudomonas aeruginosa* (>99% at 50 µg/mL) indicating broad-spectrum antibacterial activity and high potential to combat antimicrobial resistance. Furthermore, the lead compounds and their AgNPs showed strong inhibition of the biofilm formed by *B. subtilis*. The MTT assay on 3T3-L1 mouse fibroblast cells revealed no significant cytotoxicity for the synthesized compounds up to 150 µg/mL, indicating their selectivity towards bacterial cells. Taken together, this work demonstrates the rational development of amphiphilic polyphenol-based compounds and their AgNPs that exhibit broad-spectrum antibacterial and antibiofilm activity via multi-modal mechanisms.

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P-243

Core Diameter influence in NiO@Fe_3O_4 for Oxygen Evolution Reaction

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Abstract:

The oxygen evolution reaction (OER) is an electrochemical process where singlet OH^-/H_2O converts to triplet O_2, influenced by spin dynamics. However, the slow pace of this reaction hinders its efficiency in electrochemical water splitting. Although the theoretical equilibrium potential of water splitting is only 1.23V in standard conditions, a high overpotential is required due to the sluggish reaction kinetics of OER. Therefore, the development of efficient electrocatalysts for water splitting is of vital importance. The noble metal-based materials, such as Pt, IrO_2, and RuO_2, are regarded as efficient electrocatalysts for OER, however, their scarcity and high cost hinder their applications. In this study, we developed a core-shell structure of NiO@Fe_3O_4 via hydrothermal synthesis as an efficient oxygen evolution reaction catalyst. Experimental results exhibit an outstanding OER performance, with overpotential of only 94mV at a current density of 10 mA cm^{-2}. Furthermore, the 18-hour Chronoamperometry test confirmed its stability. This hetero-structural catalyst boosts the Oxygen evolution reaction due to its substantial surface area, which plays a crucial role in enabling the exposure of greater number of active sites leading to augmented contact area between catalyst and electrolyte.

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P-244

Magnetic β-glucosidase-inorganic hybrid nanoflowers: Highly active and recyclable nano-biocatalyst for cellobiose hydrolysis

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The high surface area, increased enzyme activity, active site accessibility and improved stability of the enzyme-inorganic hybrid nanoflowers have garnered significant attention in recent years. In this study, we have successfully novel magnetic β-glucosidase-Cu3(PO4)2 nanoflowers (BGL@MNFs) using the co-precipitation method. In the presence of iron oxide nanoparticles, the formed hybrid structure shows 3.5 times higher activity than in the absence of iron oxide nanoparticles and the free enzyme. Additionally, the Km value of BGL@MNFs (319.93 µM) decreased significantly compared to the free enzyme (372.25 µM), indicating the higher affinity of the enzyme towards the substrate post-immobilization. The product inhibition assay revealed that BGL@MNFs are more resistant to inhibition by glucose, even at higher concentrations. Moreover, after 10 cycles of reusability, 69.97 % glucose yield was obtained at the end of 10 reusability cycles, suggesting that the formed floral hybrid structure shows a promising way to improve the catalytic features of the enzyme.

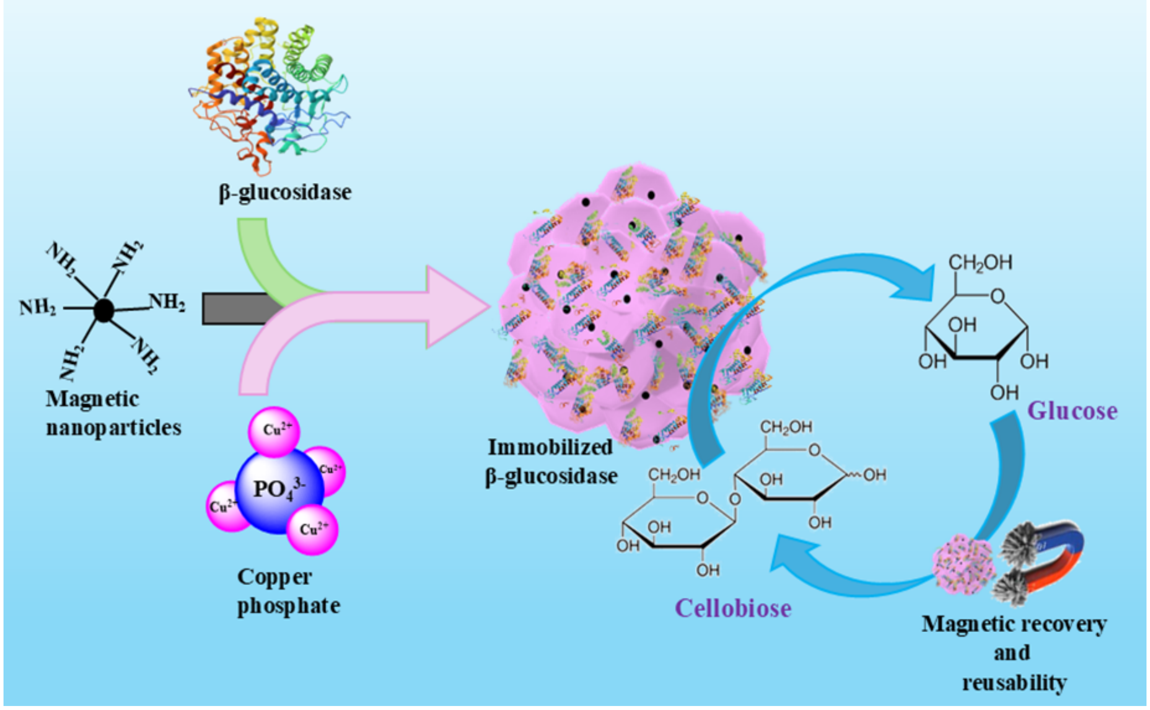

Figure 1. Graphical abstract of the magnetic hybrid nanoflowers for cellobiose hydrolysis

P-245

Electrochemical NH-Sulfoximidation with α-Keto Acids

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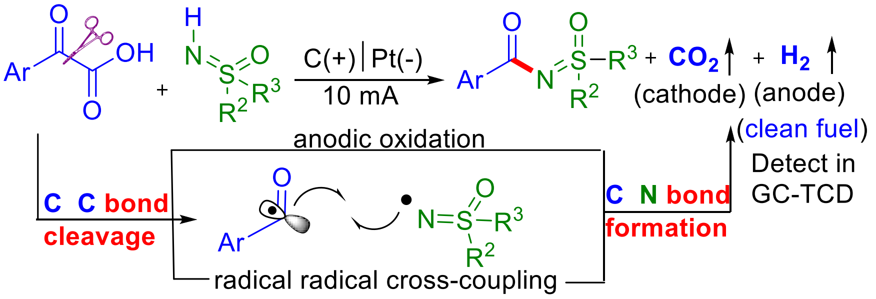
An electrochemical N-acylation of sulfoximine has been achieved via the coupling of α-keto acids and NH-sulfoximines. This process involves the sequential cleavage of C□C bond followed by C(sp^2)□N bond formation, with the liberation of H_2 and CO_2 as the by-products. A library of ***N***-aroylated sulfoximines is produced via the coupling of aroyl and sulfoximidoyl radicals by anodic oxidation under constant current electrolysis (CCE). The compatibility of the present protocol has been demonstrated by coupling of various bio-active compounds, such as NH-sulfoximine derived from (-)-borneol, L-menthol, D-glucose derivative and some commercial drugs such as flurbiprofen, and ibuprofen. This late-stage functionalization highlights the importance of this sustainable protocol. Besides this, various control experiments and detection of H_2 evolution have been performed to support the proposed mechanism.



✓ metal and oxidant-free ✓ Late-stage functionalization

✓ detailed mechanistic study ✓ quantitative analysis of clean fuel

Reference

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P-246

Ru-Catalyzed Redox-Neutral Coupling of *N*-Chlorobenzamides with Unsymmetrical Alkynes in Water

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In water Ru-catalyzed annulation of *N*-chlorobenzamides with unsymmetrical internal alkynes bearing aryl, hydroxy, ester and sulfonyl functionalities has been accomplished to afford isoquinolone scaffolds under external oxidant-free conditions at room temperature. Use of water as reaction medium, redox neutral conditions, regioselectivity and substrate scope are important practical features.

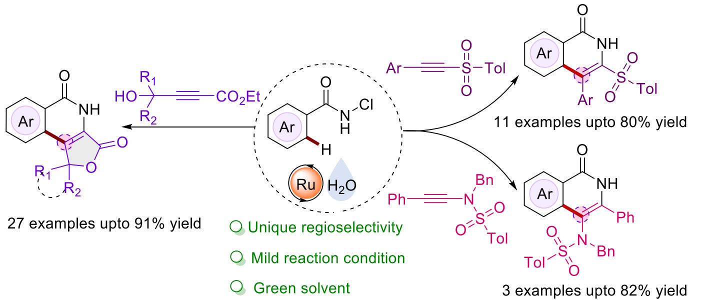

Figure 1. *N*-chlorobenzamide directed C-H activation and Annulation

The reaction of *N*-substituted benzamides with unsaturated coupling partners is a promising approach for constructing nitrogen-containing heterocyclic frameworks. However, these annulations typically depend on external oxidants and require an additional step to remove the directing group (DG).[1] Recent efforts have focused on using *N*-chlorobenzamides, where the *N*-Cl bond can function as both the DG and internal oxidant. Furthermore, annulation with alkynes is particularly appealing, as it leads to the formation of isoquinolones, which are important structural components in natural products and bioactive molecules. Developing new synthetic strategies to tackle the coupling of heteroatom-functionalized unsymmetrical alkynes is valuable because these can yield furanone-fused and heteroatom-containing isoquinolone frameworks. Additionally, using water as the solvent for C-H functionalization is desirable, as it is non-flammable, readily available and simplifies product isolation. In this work, we present a Ru-catalyzed annulation of *N*-chlorobenzamides with unsymmetrical 4-hydroxy-2-alkynoates, alkynyl sulfones and sulfonyl-based ynamides in water at room temperature.

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P-247

Biosynthesis of silver nanoparticles using *Connarus monocarpus* plant extract and its application as melamine sensor

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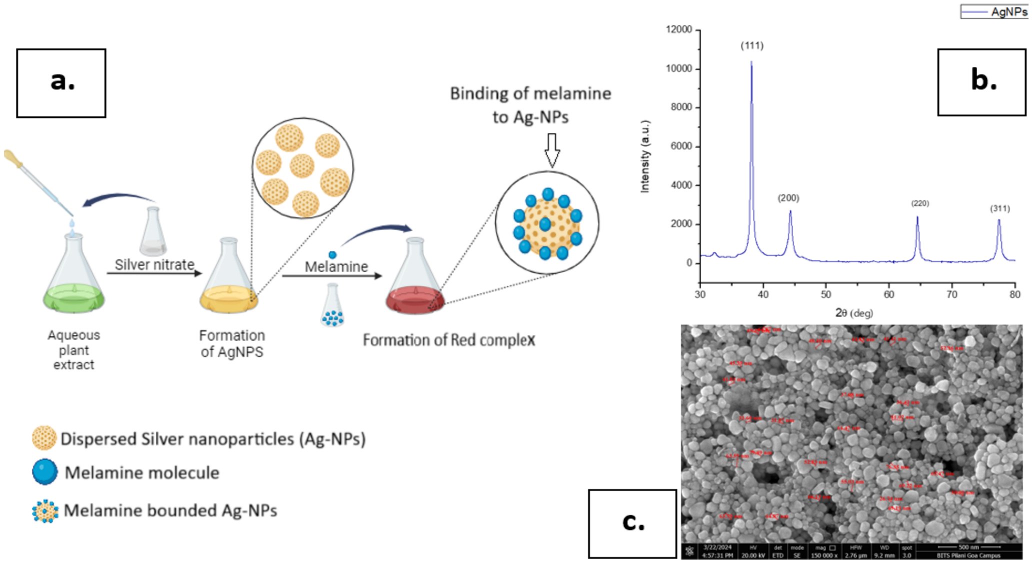
SGrowing demand for biogenic nanoparticles has been seen in recent years due to the swift advancement of nanotechnology in various fields like medicine and biology. In this work, we propose a rapid and cost-effective colorimetric sensor for detecting melamine, a common milk adulterant using biogenic silver nanoparticles synthesized using *Connarus monocarpus* leaf extract as reducing and functionalizing agent (Fig. 1 a). Optimization of the synthesis protocol was studied by exploring various parameters to yield silver nanoparticles (Ag-NPs) with average size of 100 nm. The Ag-NPs formed were characterized by UV–Visible spectrophotometer, FESEM, X-ray diffractometer, zeta sizer, DLS, EDX, Infrared and Raman spectrophotometer. X-ray diffraction studies revealed that the Ag-NPs were highly crystalline (Fig. 1 b). FESEM confirmed the formation of spherically shaped Ag-NPs and Energy-dispersive spectroscopy further verified the presence of elemental silver (Fig. 1 c). The zeta potential was found to be -23.33 mV. Dispersed Ag-NPs get aggregated upon the addition of melamine by changing the color from yellow to reddish orange due to electron donor-acceptor interactions between melamine and the nanoparticles which was confirmed by UV-Visible spectroscopy. Under optimal conditions, the Ag-NPS could selectively detect melamine within the concentration range of 1-10 ppm. In addition, the synthesized nanoparticles demonstrated significant antibacterial, anti-inflammatory, antioxidant, and anti-diabetic activities, highlighting their future in sustainable nanomedicine applications. This method doesn't generate hazardous waste due to the use of biological reducing agents proving to be economical and environment friendly.



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P-248

Analogues Copper Nanoclusters ($Cu_{16/17}$) with Two Electron Superatomic and Mixed-valent Cu^{II}/Cu^{I} and Cu^{I}/Cu^{0} Characters

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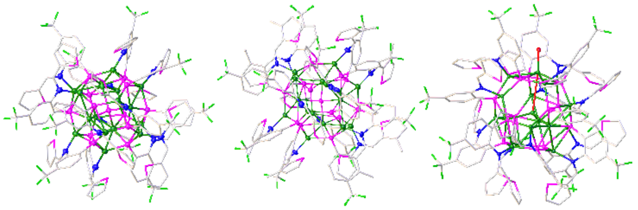
The reported copper nanoclusters (Cu NCs) having either Cu^{II}[1] or Cu^{I}[2] or mixed valence Cu^{II}/Cu^{I}[3] or Cu^{I}/Cu^{0}[4] characters are commonly observed to be stabilized by a distinct set of ligand donors. Therefore, the analogous Cu NCs with a common architecture supported by same or nearly same donor set exhibiting different mixed-valence (MV) states of Cu, such as Cu^{II}/Cu^{I} or Cu^{I}/Cu^{0}, are not yet reported. In this work, such a series of highest nuclearity copper clusters supported by aromatic thiol-S donor ligands, like $[(L4)_{12}Cu^{I}_{15}Cu^{II}(\mu_4\text{-}S)](PF_6)_3$ **(1),** $[(^{Me}L4)_{12}Cu^{I}_{15}Cu^{0}(\mu_4\text{-}S)]ClO_4.8C_7H_8$ **(2)** and $[(L4)_{12}Cu^{I}_{15}Cu^{0}_{2}(DMF)](PF_6)_3.C_2H_5OH.2C_7H_8$ (**3**), where, $^{X}L_4$=2-(3-X-thiophen)-2-yl-methylene)amino)-4-(trifluoromethyl)benzenethiol (X = H/Me), have been synthesized and their electronic structural properties have been reported. The Cu_{16} NCs, **1** and **2**, feature a central sulfido-S (S^{s}) bridged tetracopper, $S^{s}Cu_4$ core inside a sphere shaped $Cu_{12}S_{12}$ truncated octahedron. As **1** and **2** have a non-metal (chalogen or halogen) central atom (here S^{s}) instead of a metallic Cu core inside the $Cu_{12}S_{12}$ shell, these are of inverse coordination complex (ICC) [5] category, rather than superatomic with a core-shell (core is metal and shell is metal-ligand framework) structure. In presence of polar solvents, the NC **1**, gets converted to a two electron superatomic Cu_{17} NC,**3**. The NC **3** exhibits a trigonal pyramidal shaped Cu_4 core inside the modified $Cu_{12}S_{12}$ i.e. $Cu_{13}S_{12}$ shell. The transformation of **1** to **3** may be visualized as the replacement of the central sulfido-S by an extra Cu atom (generated from decomposed molecules of **1**) and shifting of a Cu atom of $S^{s}Cu_4$ unit to the $Cu_{12}S_{12}$ shell, resulting $Cu_{13}S_{12}$ shell.



1 2 3

Figure 1. The full view of the cationic part of **1**,**2** and **3** with the atoms linked to C and C atoms in wire frame (copper atoms are green, sulphur atoms are purple, nitrogen atoms are blue and the oxygen atoms are red). Cu-O(DMF) bond is also shown in **3**. The disordered F atoms of the $-CF_3$ groups, the hydrogen atoms and the counter anions are omitted for clarity.

This work furnishes the first example of (i) an ICC having Cu^{0} character (i.e. **2**), (ii) an aromatic thiol-S donor ligand stabilizing superatomic Cu NC (i.e.**3**), (iii) the spontaneous conversion of ICC (i.e. **1**) to superatomic NC (i.e. **3**) that does not require any reducing agent rather occurs in presence of dioxygen oxidant. To the best of our knowledge, the presence of S^{s} in **1** and **2** discloses the first evidence of the benzene thiol C-S bond cleavage. The spectroelectrochemical studies elucidated the selection of Cu^{II}/Cu^{I} and Cu^{I}/Cu^{0} character of **1** and **2** respectively which are further supported by the high resolution XPS and Cu- LMM spectroscopy.

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P-249

Visible-light promoted Synthesis of Schiff Base via C-N bond formation: Benzyl Alcohol as an alternative of Aryl aldehydes

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The development of photocatalytic methods has opened the way for green chemical synthesis using visible light-induced photochemical oxidation under mild conditions. Here, a new strategy utilizing Eosin-Y as a catalyst under visible light has been introduced for the reaction between substituted benzyl alcohols and anilines, leading to the formation of various Schiff bases. This method stands out for being environmentally friendly, metal-free, cost-effective, and non-toxic.

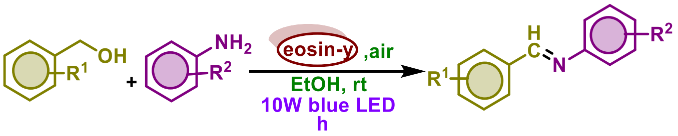

Figure 1. Visible light promoted synthesis of Schiff base from benzyl alcohol and aniline.

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P-250

MnO_2/PPy Hybrid Electrode; Advanced High-Performance Supercapacitors

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The increasing global demand for renewable energy technologies has sparked extensive research efforts aimed at addressing the rapid depletion of fossil fuels and their negative environmental impacts. To support the transition to sustainable energy, there is an urgent need for efficient, cost-effective energy storage devices capable of storing and delivering energy reliably. Supercapacitors have garnered significant attention as vital components in modern energy storage systems due to their high power density, rapid charge/discharge rates, and excellent cycle stability. However, their relatively low energy density remains a major limitation for broader practical applications. Various strategies have been explored to enhance energy density, including the use of transition metal oxides. Among these, manganese dioxide (MnO_2) stands out due to its high theoretical capacitance, abundance, low cost, and environmental friendliness [1]. Despite these advantages, MnO_2 suffers from poor electronic conductivity, which hinders its practical capacitance. To overcome this, fabricating composite electrodes by incorporating conductive materials is a promising solution. Conducting polymers, such as polypyrrole (PPy), are particularly attractive due to their high pseudocapacitive properties and good electrical conductivity [2]. PPy's synergy with MnO_2 makes it an ideal candidate for boosting the overall energy density of the electrode. In this work, we fabricated MnO_2/PPy hybrid electrodes via an electrodeposition technique. The surface morphology of the MnO_2/PPy composite was characterized using scanning electron microscopy (SEM), while Fourier transform infrared (FTIR) spectroscopy was used to analyze functional groups. Raman spectroscopy was employed to further establish the uniform coating. Electrochemical performance was evaluated using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). The MnO_2/PPy hybrid electrode demonstrated superior electrochemical properties, making it a promising candidate for high-performance energy storage applications.

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P-251

Analysis of Physicochemical Parameters of Ground water around Silapathar and Simen Chapori Area of Dhemaji district, Assam

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In Assam, for a rural district like Dhemaji, where the majority of the people live below the poverty line (BPL), the facility of drinking water is one of the requiring conditions for good health and all-round development. Several researchers have studied physico-chemical parameters of groundwater in selected areas of rural and sub urban areas of Dhemaji district. From the literature review, Buragohain et al. presented a statistically significant water quality database of Dhemaji district, Assam (India) with special reference to pH, fluoride, nitrate, arsenic, iron, sodium and potassium. [1, 2, 3] But none have investigated the various parameters of ground water of Silapathar and Simen Chapori area of Dhemaji district. In this background, we have planned to instigate this work which is locally relevant and has lab to land orientation as well. Since the levels of certain physico-chemical parameters like pH, alkalinity, BOD, COD, total hardness, Ca, Mg, Chlorides, HCO_3^-, CO_3^{2-}, NO_3^-, PO_4^{3-}, Na, K, heavy metals and total dissolved solids found in ground water determine its demeanor as well as quality, it has been proposed to evaluate ground water in different areas separately so as to find reasons for the ground water problems in the said area. All over study represents that some of samples have poor quality for consumption and required regular monitoring for avoid further contamination. From our study, it is observed that some of the samples are safe for drinking purpose. But, in case of the samples having high iron content, the people should use filter for safe drinking water. There is a rising risk of groundwater contamination not only in urban areas but also in rural areas. To alleviate the risk of further groundwater contamination and improve groundwater quality, the following recommendations can be concluded.
(a) quality of groundwater sources i.e. dug wells and boreholes, should be regularly examined in both urban and rural communities and proper awareness should be made to their residents on the condition of their groundwater resources;
(b) efficient, economical and environmentally-friendly sewerage systems should be designed.

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P-252

A carbon nanodot-based torch for detecting carbon monoxide

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Carbon monoxide (CO), a prevalent environmental pollutant, accounts for a large percentage of accidental poisonings and fatalities reported worldwide each year. Precise detection and control of CO in residential and industrial environments are essential to reduce the risk of serious health issues in humans, owing to its toxic properties and numerous sources. [1-3] CO is colorless, odorless, tasteless, and non-irritating, making it particularly difficult to detect without specialized equipment. [4] In this study, we have developed a portable sensor utilizing nitrogen-doped carbon quantum dots (N-CQDs) to detect atmospheric CO at any location (Figure 1). It is designed for real-time monitoring in a wide range of environments. In this detection process, we utilized the fluorescence quenching mechanism of N-CQDs upon interaction with CO, achieving a detection limit of 0.102 µM. Various analytical techniques, such as Dynamic Light Scattering (DLS), Energy Dispersive X-ray Spectroscopy (EDX), Fourier-transform Infrared Spectroscopy (FT-IR), X-ray Photoelectron Spectroscopy (XPS), UV-visible spectroscopy, fluorescence spectroscopy, and fluorescence lifetime decay, were employed to elucidate the quenching mechanism.

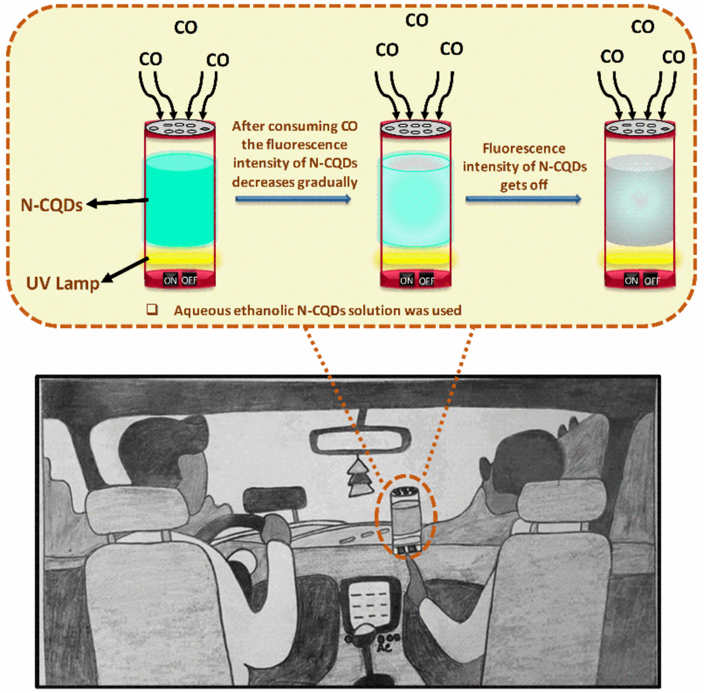

Figure 1. Diagrammatic illustrations of the device engineered for real-time CO detection across various environments.

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P-253

Highly conductive multifunctional Iron incorporated Polythiophene nanocomposite: A nanocatalyst for nitrobenzene reduction in aqueous medium and an efficient room temperature methanol gas sensor

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Multifunctional composite particles have received considerable attention because of their potential applications, such as biomedical, catalytic, electromagnetic, and sensing. PTh-Fe^0-Fe_2O_3 nanoparticles with multi-functionality (i.e., catalytic and gas sensing) were successfully fabricated via in- situ polymerization. Nitrobenzene (NB) is among the commonly exploited pollutant mainly in oil refinery wastewaters. To introduce a potential reducing agent for the removal of NB, herein a novel type of magnetic nanocatalyst so-called Polythiophene-Iron (PTh-Fe^0-Fe_2O_3) have been successfully synthesized. Fe^0-Fe_2O_3 nanoparticles were synthesized using tea leaf extract as the reducing agent .The prepared nanocatalyst has good catalytic activity in the selective nitro- group reduction of nitroarenes and can be regain by external magnet and recycle several times.The simple operation, use of inexpensive and benign iron NPs coated Polythiophene as reducing species, no requirement of conventional co-reducing agent, mild reaction conditions of room temperature and aqueous medium, short reaction time, high yields of amines and, above all, the unique chemoselectivity make this procedure an unique choice for reduction of aromatic nitro compounds. Again, the sensitivity of the PTh-Fe^0-Fe_2O_3 sensor to different concentrations of Methanol gas was investigated at room temperature. The experimental results showed that the PTh-Fe^0-Fe_2O_3 nanocomposite shows excellent performance in terms of high response and selectivity: the sensitivity (%) at 200 ppm methanol was found to be as high as 52.6 %, which was clearly superior to that found for pristine PTh. The PTh-Fe^0-Fe_2O_3 nanocomposite showed excellent sensitivity towards methanol sensing, which can be attributed to the interaction between p-n heterojunctions in the magnetic nanocomposite.

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P-254

A ratiometric luminescent Tb(III) complex for efficient sensing of anthrax biomarker "DPA"

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Lanthanide coordination complexes have emerged as an important class of luminescent materials possessing practical applications in various fields such as catalysis, gas storage, separation, magnetism, drug delivery etc.[1] Due to the Laporte forbidden 4*f*-4*f* transitions, direct photoexcitation of lanthanide ions is difficult. Therefore, organic ligands play an important role in enhancing luminescent properties of lanthanide ions through "Antenna-effect".[1] Herein, we report a bimetallic Tb(III) complex, which has been synthesized by solvothermal method. The resulted complex was successfully characterised by elemental analysis, FT-IR, Powder-XRD, thermogravimetric analysis and X-ray crystallography. Further, the applicability of the complex in luminescence sensing was studied.

At λ_{ex}= 266 nm, the Tb^{3+} complex flaunts four weak characteristic emission peaks, with the most notable peak at 544 nm, indicative of the characteristic green luminescence of Tb^{3+} ions, alongside a strong ligand emission centered at 358 nm. The weak emission bands are due to the inefficient sensitization of Tb^{3+} ions by the ligands. This prompted us to investigate the sensing properties of DPA, a biomarker for anthrax that effectively sensitizes Tb^{3+} metal ions.[2] The Tb(III) complex demonstrated a highly sensitive, self-calibrating ratiometric response for detecting DPA. Specisfically, the LC emission band at 358 nm displayed a decrease in fluorescence intensity upon the addition of DPA, while the emission intensity at 544 nm increased, resulting in a limit of detection (LOD) value of 6 μM, significantly lower than the threshold dose of DPA for human infection (60 μM).[3] Furthermore, the capability of complex to detect DPA was validated with real samples, yielding remarkable results. Therefore, the synthesized complex holds promise for effective and reliable ratiometric sensing of the anthrax biomarker in practical scenarios.

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P-255

Microwave Assisted Syntheses of Indolo[2,3-*b*]quinoline Scaffold containing heterocyclic compounds and the Alkaloid Neocryptolepine.

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Indoloquinoline alkaloids, featuring fused indole and quinoline rings, are rare but biologically active compounds.[1] They are mainly found in the climbing vine *Cryptolepis sanguinolenta* (Lindl.) Schltr (Asclepiadaceae), of West and Central Africa, locally known as nibima, kadze, and gangamau.[2] Till date 16 indoloquinoline alkaloids have been isolated from the plant.[3] Neocryptolepine or 5-methyl-5*H*-indolo[2,3-*b*]quinoline, a tetracyclic nitrogen heterocycle, is notably studied for its potential in treating various diseases due to its antibacterial, antimalarial, antiproliferative, antischistosomal, and antiplasmodial properties.[1-4] The primary objective of this study was to synthesize indolo[2,3-*b*]quinoline using microwave irradiation as an eco-friendly method. The approach aimed to achieve shorter reaction time, reduced temperature, and improved yields.

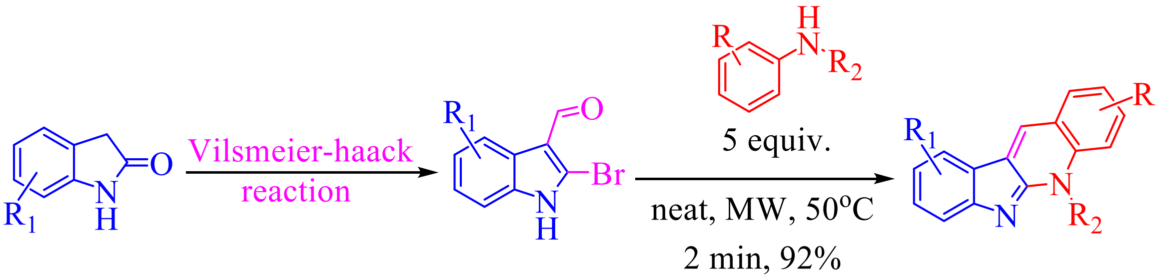

Figure 1. Graphical abstract of the microwave-assisted synthesis of Neocryptolepine.

We have successfully synthesized indolo[2,3-*b*]quinoline scaffold using microwave irradiation as an environmentally friendly method. The structures of the synthesized compounds were confirmed through spectroscopic techniques. The reported protocol (**Figure 1**) presents significant advantages over conventional methods for synthesizing indolo[2,3-*b*]quinoline.[5] It requires substantially less reaction time and operates at lower temperatures compared to traditional reflux methods. Additionally, the yield achieved with this protocol is markedly higher than that obtained using conventional techniques. We were also successful at synthesizing some novel derivatives of neocryptolepine with excellent yields.

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P-256

Multiferroic $BiFeO_3$ nanoparticles as an efficient photocatalyst for sunlight-driven photocatalytic removal of textile dyes

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In recent decades, semiconductor-assisted photocatalysis has gained significant attention for the treatment of dye-contaminated wastewater due to its high selectivity, efficiency, and environmental friendliness [1]. Among the promising materials, bismuth ferrite (BFO) has emerged as a leading candidate for photocatalytic applications under visible light. Its appeal lies in its unique multiferroic properties, along with a narrow bandgap, excellent chemical stability, and non-toxicity. This study presents a simple and cost-effective sol-gel method for synthesizing phase-pure BFO nanoparticles (NPs) using propylene glycol as a complexing agent.

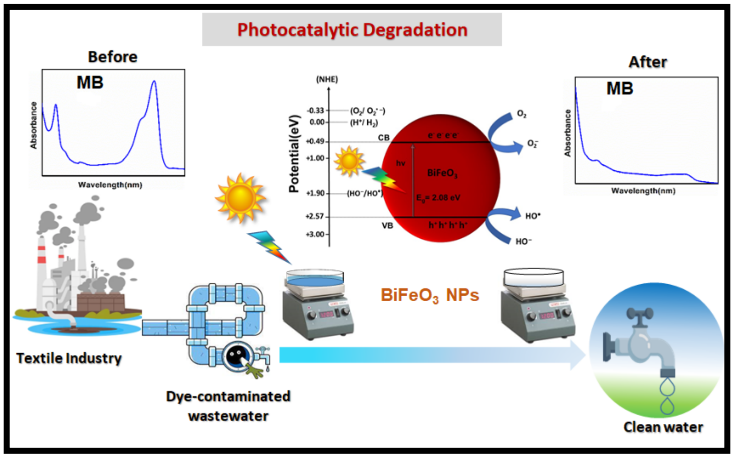

Figure 1. Graphical abstract of the Photocatalytic Degradation process

Synthesized BFO NPs were characterized by TGA, FT-IR, XRD, TEM, Raman. Rietveld refinement of XRD data, combined with TEM and Raman spectroscopy, confirmed the successful synthesis of phase-pure BFO NPs at 400°C, exhibiting an average crystallite size of about 25 nm and a space group of R3c. UV-visible DRS revealed an absorption cutoff at 590 nm, corresponding to a bandgap of 2.08 eV, demonstrating the ability of BFO NPs to absorb visible light in the 400-590 nm range. The photocatalytic performance was evaluated by degrading methylene blue (MB) dye under various pH conditions (acidic, neutral, and basic) using natural sunlight. The enhanced photocatalytic activity is attributed to the intrinsic ferroelectric and ferromagnetic properties of BFO NPs, which facilitate efficient separation and migration of photo-induced charge carriers via band bending at the material's surface [3].

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P-257

Cost-effective Computations of Gold Standard of Quantum Chemistry

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Quantum chemical (QC) methods play a crucial role in understanding the structures, energetics, and vibrational features of molecular systems. However, *ab initio* treatment of large systems remains limited due to the inherent non-linear scaling of QC methods, especially for the correlated level investigations.[1] Fragmentation approaches based on the divide-and-conquer strategy offers a cost-effective solution for bypassing the full conventional calculations (FC) on large molecular systems at correlated levels of theory using extended basis sets.[2] The Molecular Tailoring Approach (MTA), one such approach is certainly useful for efficient computations on off-the-shelf harwdare.[3]

The current study represents a state-of-the-art protocol for enabling CCSD(T) level energetics, famously known as contemporary gold-standard of quantum chemistry, for a variety of molecular systems comprising of covalent systems (H_2O, CO_2, and NH_3 clusters) and non-covalent systems (glycine, traumatic acid, and *cis*/*trans*-sphingenine). From the comparison with FCs wherever feasible, MTA shows remarkable accuracy and efficacy on limited hardware. Further, a comparison is also made between the MTA-derived results and the results derived from the Fragment Molecular Orbital (FMO) method at similar levels of theory.[4]

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P-258

A Recyclable MOF@polymer Thin Film Composite for Nanomolar On-Site Fluorometric Detection of Heavy Metal Ion and Anti-Histamine Drug

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The toxicity of mercury has been recognized for centuries with historical records describing its harmful effects on miners and artisans exposed to fumes and vapours.[1] Ranitidine is a widely used medication belonging to histamine-2 receptor antagonists.[2] Its improper disposal or presence in wastewater can contaminate groundwater, posing risks to drinking water sources. Additionally, the use of ranitidine has been associated with the development of antimicrobial resistance. Developing a robust, reliable, fast-detecting sensor is a significant challenge for present-day researchers. In this work, a dual-functional fluorometric sensor was designed to detect heavy metal ions (e.g., Hg^{2+}) and anti-histamine drugs (e.g., ranitidine) at the nanomolar level in the aqueous medium. A stable and efficient thiourea-functionalized aluminum−based metal-organic framework (**1**) was prepared and its guest-free form was applied for the selective detection of the above-mentioned analytes with a low detection limit (Hg^{2+} = 7.3 nM and ranitidine = 3.4 nM). The MOF was exceptionally sensitive to Hg^{2+} and ranitidine detection with a fast response time of 10 s and 5 s, respectively. Our probe has the highest KSV values for these targeted analytes among the sensors documented to date (i.e., 1.29 × 106 M^{-1} for Hg^{2+} and 7.99 × 105 M^{-1} for ranitidine). This work reports the first MOF-based sensor for ranitidine detection. About 93% and 98% fluorescence quenching was observed after introducing Hg^{2+} and ranitidine, respectively. The probe has excellent selectivity toward detecting Hg^{2+} and ranitidine, even in the presence of interfering analytes. The sensing capability of the probe was explored in different media, including serum, urine, wastewater, different pH, etc., which indicates the real-field applicability of the sensor. A cost-effective, highly efficient, long-lasting MOF@polymer thin-film composite (MOF@PVDF-PVP) was employed for the on-field qualitative detection of Hg^{2+} and ranitidine. The mechanistic insights into the sensing were well explored with the help of different modern analytical techniques. The ground-state complexation and inner filter effect were responsible for fluorescence quenching in the presence of Hg^{2+} and ranitidine, respectively.

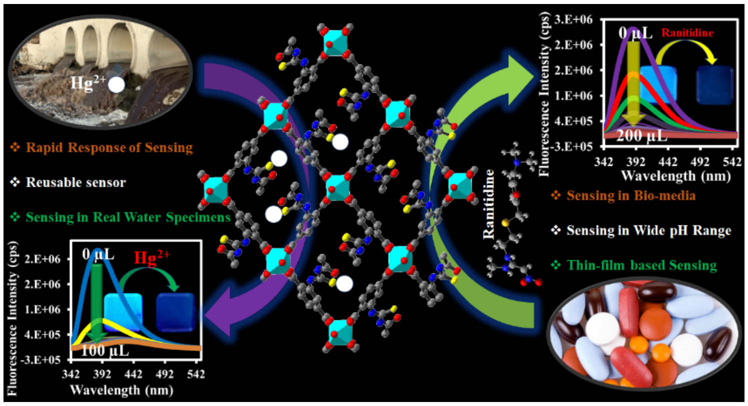

Figure 1. Graphical abstract for fluorometric monitoring of Hg^{2+} and ranitidine using the probe **1**.

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P-259

Impact of Dopant Concentration on the Growth Kinetics of Carbon Nanotubes

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Carbon nanotubes (CNTs) are cylindrical, one-dimensional structures made of sp^2 hybridized carbon atoms arranged in hexagonal lattices. Since their rediscovery, CNTs have garnered significant attention due to their exceptional properties. Modifying the sp^2 carbon lattice by incorporating heteroatoms can tailor their physicochemical properties, broadening their potential applications. In this study, boron-doped carbon nanotubes (BCNTs) were synthesized using the Floating Catalyzed Chemical Vapor Deposition (FCCVD) method, with ethanol, boric acid, and ferrocene serving as the carbon (C), boron (B) sources, and catalyst precursor, respectively. The doped CNTs were characterized using Raman spectroscopy, Field Emission Electron Scanning Microscopy (FESEM), and X-ray photoelectron spectroscopy (XPS). Reaction kinetics were studied across a temperature range of 800-1000°C with varying dopant concentrations. It was found that increasing dopant concentration led to a decrease in reaction rate. The activation energy of the reaction at different dopant concentrations was found to be 36 $kJmol^{-1}$, 27 $kJmol^{-1}$, 47 $kJmol^{-1}$ and 73 $kJmol^{-1}$ respectively. Raman spectra revealed both the D-peak (indicative of defects) and the G-peak (representing graphitic structure), with an I_D/I_G ratio ranging from 0.63 to 1.02. XPS analysis confirmed boron incorporation, showing boron atomic percentages of 1.78-2.75%. FESEM images displayed CNT bundles with diameters ranging from 40-80 nm. This study offers important insights into the kinetics of doped CNT growth, which is essential for scaling up the synthesis process.

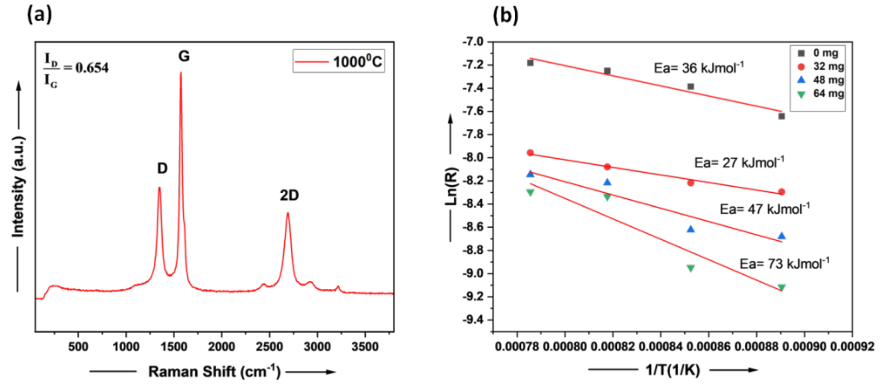

Figure 1. (a) Raman spectra of boron-doped material synthesized at 1000⁰C and (b) Arrhenius plot at different dopant concentrations.

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P-260

End group modulation of A-D-A type small donor molecules for DTP based organic photovoltaic solar cells: A DFT approach

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The primary objective of the 21st century is to develop clean and renewable energy technologies. Key renewable sources include solar, tidal, wind, biogas, and hydro energy.[1] In this context, solar energy stands out as a viable option due to its renewability and environmental safety.[2] Increasing energy demand and environmental concerns have spurred research into solar energy conversion. Photovoltaic systems and solar cells convert sunlight into electrical energy.[1] Photovoltaic solar cells can be classified into three types: inorganic solar cells using silicon, organic solar cells (OSCs) made from polymers and small acceptor molecules, and hybrid solar cells that combine organic and inorganic materials.[3] Among them, OSCs have gained significant interest in recent years due to their cost-effectiveness, mechanical flexibility, solution processability, lightweight nature, and aesthetic appeal.[4] This presentation will review our efforts to develop new effective materials as potential candidates for OSC fabrication.

Firstly, we have designed five A-D-A type small donor molecules, C1-C5, with DTP as the central donor unit.[5] The end-group acceptor units for C1-C5 are 1,1-dicyano-methylene-5,6-dimethyl-3-indanone, 1,1-dicyano-methylene-5,6-difluoro-3-indanone, 1,1-dicyano-methylene-5,6-dichloro-3-indanone, 1,1-dicyano-methylene-5-nitro-3-indanone, and 1,1-dicyano-methylene-5,6-diamino-3-indanone, respectively. Thereafter, we have investigated the role of these small molecule donors in charge transfer processes at the donor/acceptor (D/A) interface, using C_{60}-CN as the standard acceptor.[6] Employing density functional theory (DFT) and time-dependent density functional theory (TD-DFT), we have analyzed the structural and optoelectronic properties of the designed compounds. The study indicates that our compounds have the potential to serve as donor materials for OSC fabrication.

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P-261

$NiFe_2O_4$@Chitosan-Anchored Magnetically Retrievable Cu(II) Schiff Base Complex: A versatile catalyst for Multicomponent Reaction

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We reported, herein, the fabrication of Cu(II) Schiff base metal complex, immobilized on chitosan surface coated with nickel ferrite MNPs, intented as a novel heterogeneous and magnetically recyclable nanocatalyst, $NiFe_2O_4$@CS@CuSB. Through comprehensive characterization of the prepared nanocatalyst using FT-IR, PXRD, SEM, EDS, TEM, SAED, VSM, BET and XPS, the structure, surface morphology, elemental composition and characteristics of the catalyst are revealed. For the evaluation of its catalytic activity, $NiFe_2O_4$@CS@CuSB, has been utilized as a potential nanocatalyst for the one-pot multicomponent organic synthesis of 1-amidoalkyl-2-naphthol scaffolds (Fig.1). A straightforward, effective, one-pot, and environmentally safe synthesis of 1-amidoalkyl-2-naphthol has been accomplished using a broad range of aldehydes, 2-naphthol, urea, or amide, demonstrating the catalyst's strong resistance to different functionalities. High yields of the intended products have been obtained without the formation of byproducts. A hot filtration test was employed to evaluate the heterogeneity of the solid nanocatalyst. With potential uses in medicinal chemistry, this novel catalyst presents a viable method for the effective production of bioactive molecules.

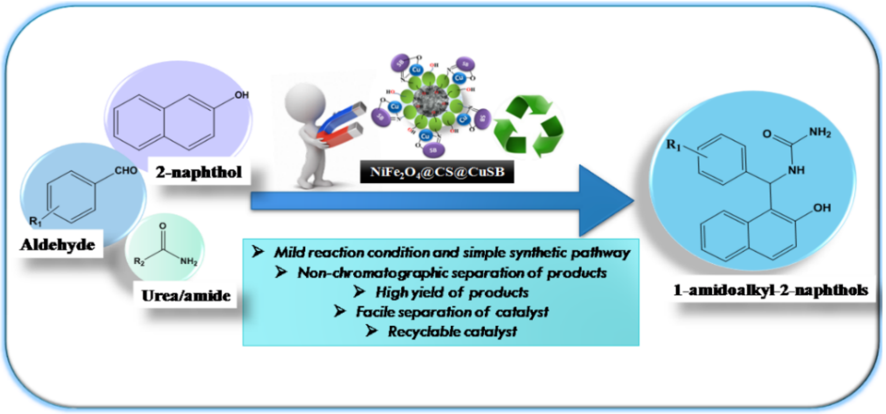

Figure 1: Graphical abstract for catalytic activity of $NiFe_2O_4$@CS@CuSB in multicomponent reaction

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P-262

Enhanced Performance of πconjugated Metal Complex (TPZn) in Organic Field Effect Transistors

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The self-assembled layers especially nanolayers obtained from various functional л-conjugated organic imperative for fabricating organic devises like organic field effective transistors (OFETs), optoelectronic devices, organic field effective transistors (OLEDs). Therefore, understanding the π-conjugation becomes one of the most important research areas in the molecular electronics. To achieve this goal, in this study, we have designed and synthesized a functional property for improved performance in OFETs by using ϖ-conjugated molecule with metal complex (TPZn) having phenanthrol[9,10-d] imidazole with terpyridine substitution. The PVDF with N,N Dimethylacetamide is used as a dielectric material. Where the β-phase is formed, and it has been confirmed with FTIR. The phenanthrol[9,10-d] imidazole, especially the 2-substituted ones, have been extensively used as luminescent sensors and OLEDs. On the other hand, we have investigated results with density functional theory (DFT) studies, which clarifies the π-conjugation system of (TPZn) impacts the energy levels, which is responsible for multiple charge transfer properties. DFT calculations were performed to corroborate the experimentally obtained results on the solvent polarity-induced tuneable optical properties. Furthermore, the most important characteristics of electronic device can be appraised by the current and current density-voltage (I&J-V) measurements exploited to examine the material properties such as conductivity, charge carrier mobility and charge injection efficiency. Also, we have investigated the I-V characteristics of TPZn to evaluate their possible potential utility in electronic device fabrication. We found that the TPZn possesses better electrical conductivity or charge transport properties, which are essential for organic electronic applications.

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1. Polarity-Induced Morphological Transformation with Tuneable Optical Output of Terpyridine–Phenanthro[9,10-*d*] imidazole-Based Ligand and Its Zn(II) Complexes with *I–V* Characteristics DOI: 10.1021/acsomega.3c06283

P-263

Synthesis of Functionalized Tetralones and Naphthoquinones *via* Tamura Cycloaddition of Rauhut-Currier (RC) adducts of nitroalkenes with homophthalic anhydrides

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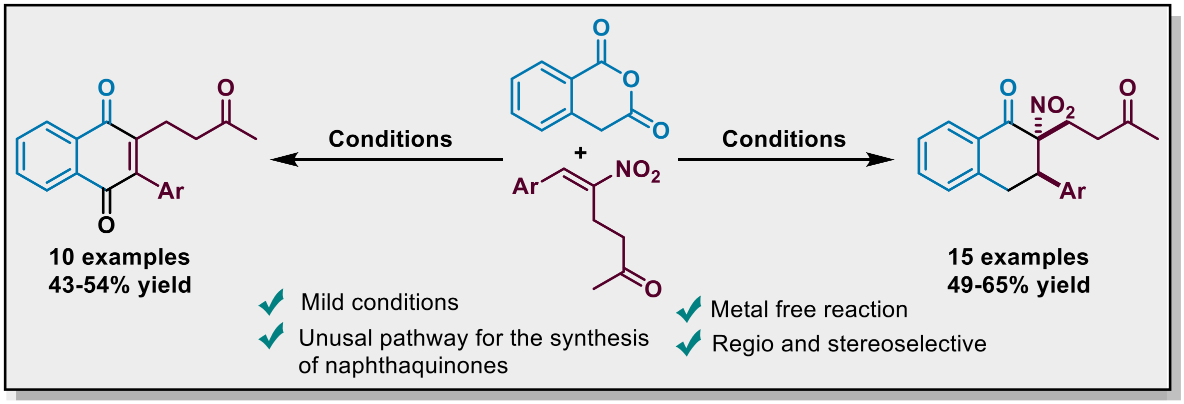
Tetralone and its derivatives are essential structural scaffolds for potential therapeutic applications.[1] It is present in different biologically active molecules and exhibits properties such as antibacterial, antifungal, anti-inflammatory, and anticancer *etc*.[2] Moreover, the noteworthy framework of naphthoquinone shows activity against Alzheimer's disease and is also present in the core structure of diverse pharmaceutically relevant molecules *etc*.[3] The synthesis of functionalized tetralones and naphthaquinones in one pot is always challenging. Our group actively engaged in the synthetic development of various methodologies using different nitroolefins. In this study, we have employed the Rauhut-Currier adduct of nitroalkene and homophthalic anhydride and demonstrated the synthesis of functionalized tetralone and naphthoquinones scaffolds by Tamura cyclization, facilitating *via* [4+2] annulation reaction. We have developed two distinct conditions to synthesize the naphthaquinones in good yields, while the tetralone scaffolds have been successfully constructed in good yield and as a single diastereomer. Moreover, those skeletons demonstrate further cyclization either in a *C*-centered or *N*-centered pathway depending upon the reagents employed.[4]



Scheme: Synthesis of tetralones and naphthaquinones from Homophthalic anhydride and Rauhut-Currier adducts of Nitralkenes

Keywords: Homophthalic anhydride, Rauhut-Currier adduct of nitroalkene, Tamura cyclization.

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P-264

Fabrication of Robust Forward Osmosis Membrane by Assembling Weakly Magnetic FeO_xCl_y Nanoparticles

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Owing to its inherent advantages like low-energy consumption, low-fouling propensity, and high recovering ability over high-pressure-driven membrane processes, the future of membrane technology is shifting towards forward osmosis (FO)[1]. However, the utility of FO in challenging areas is hindered by the lack of suitable FO membranes[2]. Here, we report the development of innovative FO membranes by depositing weakly magnetic and positively charged FeO_xCl_y nanoparticles on a negatively charged nylon membrane (FeO_x-Nyl). Remarkably, the FeO_x-Nyl membrane possesses outstanding stability in an aqueous medium and survived in both acidic (pH = 2.3) and basic (pH = 6.9) solutions for more than 7 months. Upon varying the loading amount of FeO_xCl_y, the water flux of the FeO_x-Nyl membrane varies from 27.8 to 61.3 LMH (from 5 to 30 mg). Due to its hydrophilic nature, the FeO_x-Nyl membrane exhibits excellent flux recovery rates (FRR), up to ~ 70 %. The outstanding robustness and high flux of FeO_x-Nyl were exploited in challenging applications like recovering reactive chemical wastes and dehydration of acetic acid.

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P-265

Influence of Zn substitution into Ni-Co ferrite system and study its Structural, Magnetic and Supercapacitance properties

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Nanoparticles of $Ni_{0.5-x}Zn_xCo_{0.5}Fe_2O_4$ (x=0.0-0.5) are prepared by combustion method using succinic acid as fuel. The structural, magnetic and supercapacitance properties were studied for the synthesised 'as prepared' zinc substituted Ni-Co ferrites. The XRD pattern of the 'as prepared' ferrites showed formation of monophasic cubic spinel structure (Fig.1a). There is an increase in the lattice parameter with an increase in zinc concentration [1]. The IR spectra depict two characteristic absorption peaks of spinel at around 600 cm-1 and 400 cm-1 [2].

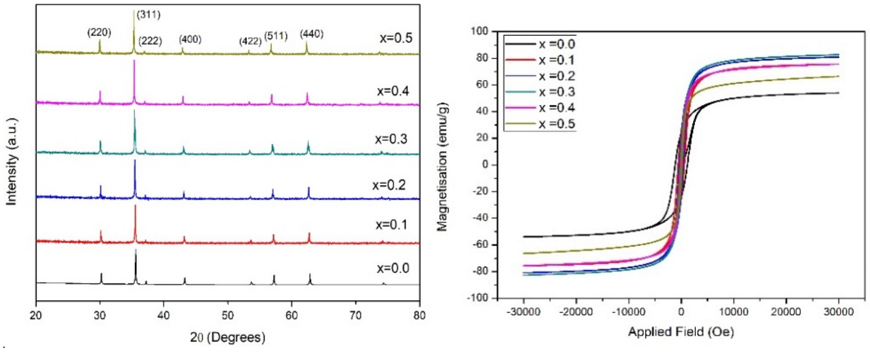

Figure 1. a) X-Ray diffraction pattern of 'as prepared' $Ni_{0.5-x}Zn_xCo_{0.5}Fe_2O_4$ (x=0.0- 0.5) and b) The VSM plots of magnetic moment against magnetic field at room temperature of 'as prepared' $Ni_{0.5-x}Zn_xCo_{0.5}Fe_2O_4$ (x=0.0- 0.5).

The Curie temperature determined from A.C. susceptibility measurements found to decrease with increase in zinc content [1]. The VSM plots of all the ferrites indicate ferromagnetic nature (Fig.1b) and shows a random trend in saturation magnetisation (Ms) with increase in the zinc content in Ni-Co ferrites may be due to variation in particle size of the end products [3]. HR-TEM images shows the agglomeration of irregular cuboidal-shaped particles. The histograms confirm that the average particle size falls within 10-45nm range [4]. The Raman spectra shows the five Raman active optical modes A1g, Eg, 2T2g as seen in ferrites. The XPS studies verified the expected oxidation states of all the corresponding elements in ferrites. The electrochemical analysis exhibited the highest capacitance (Csp) of 35.46 F/g for the composition x=0.0 at the lowest scan rate [4].

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P-266

Synthesis of CF_3CH_2-Amides/Propiolamides/Acrylamides: The TfOH Catalyzed Reactions of Nitrile Compounds with CF_3CHN_2

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Fluoroalkylation is a highly effective method for producing fluorinated bioisosteres, which have many desirable properties like improved bioavailability, metabolic stability, membrane permeability, electronegativity, and oxidation resistance.[1] While substantial efforts have been devoted to trifluoromethylation reactions, its homologous trifluoroethylations are relatively less explored.[2] In this regard, 2,2,2-trifluorodiazoethane (CF_3CHN_2) works as a convenient trifluoroethylating reagent, as its *in-situ* generation in organic solvents is safe. Furthermore, it displays multidimentional reactivity, *i.e.* it may undergo cycloaddition pathways such as [3+2], [3+3], and [2+1] with unsaturated systems.[3]

Recently, our group has documented a greener and chemoselective protocol for the trifluoroethylation of oxindoles, thioxindoles and isoindolines using CF_3CHN_2 as the trifluoroethylating reagent.[4] Further exploring the reactivity of CF_3CHN_2, herein we are demonstrating an efficient and operationally simple protocol to access *N*-(2,2,2-trifluoroethyl)amides/propiolamides and acrylamides from easily accessible nitriles (aryl/alkyl/alkynyl/vinyl) and *in situ* generated CF_3CHN_2 as trifluoroethylating reagent (Figure 1). The protocol offers broad functional group tolerance under mild reaction conditions. Furthermore, the conversion of trifluoroethylated propiolamide into its triazole analog via Ru-catalyzed [3+2] cycloadditions using BnN_3 clearly indicates its versatility in the synthetic applications.[5]

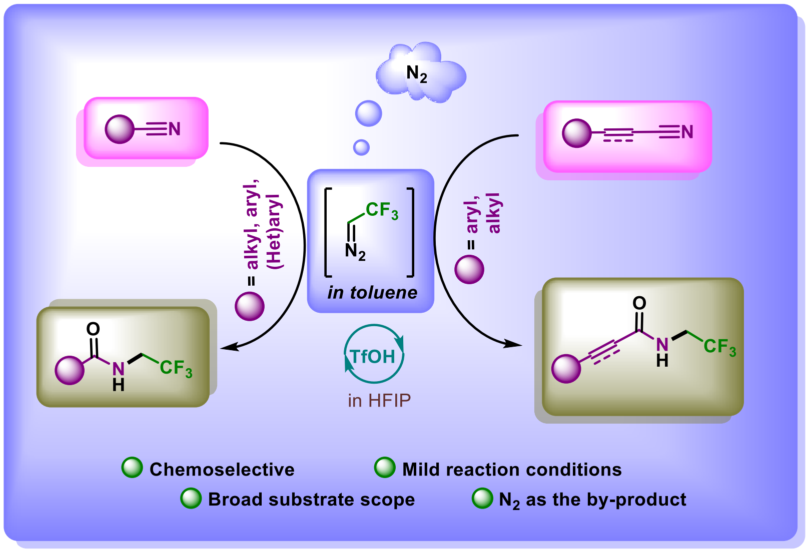

Figure 1. One step access to (2,2,2-trifluoroethyl)amide units from nitriles

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P-267

Synthetic Ion Transporter and its therapeutic application

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Signal transduction across cellular membranes is crucial for regulating various physiological processes. Membrane-embedded proteins are essential for transporting signalling molecules, and mimicking these chemical communication systems holds potential for applications in biosensing, intercellular communication, and the creation of artificial cells. Here, we describe the development of a vesicle-based system that can selectively transport ions across a lipid bilayer. The system utilizes synthesized molecules that self-assemble into ion channels, enabling controlled ion transport. This selective ion transport also triggers the formation of a catalytic system within the vesicle, which can convert non-fluorescent substrates into fluorescent products, allowing for the detection and amplification of signals. Such systems are capable of functioning as logic gates, translating chemical signals into optical outputs, similar to natural cellular processes. This work demonstrates the potential of vesicle-based molecular communication systems in replicating the complexity of biological signalling, providing new opportunities for designing biomimetic tools and understanding the principles of cellular communication.

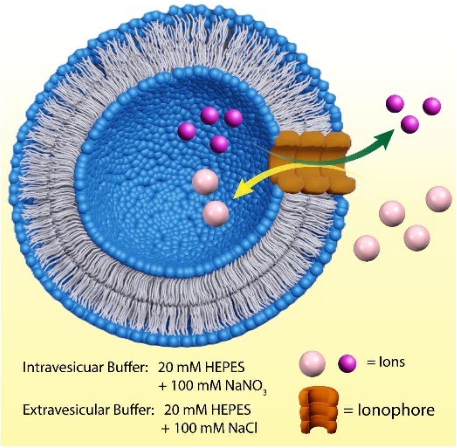

Figure 1. Graphical representation of ion transport across cellular membrane by synthetic ion transporter.

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P-268

Nitrogen and Sulfur co-doped Carbon Quantum Dot decorated $Ti_3C_2T_x$-MXene as electrode material for high-performance symmetric supercapacitors

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Considering the huge consumption of fossil fuels and cumulative energy demands in the high-tech society, energy storage devices particularly the supercapacitors take the pivotal role to explore the alternative source of renewable energy sources. To focus on the potential supercapacitor electrode material, the essential features of material are large surface area, good conductivity, and large number of active sites. Therefore, the integration of a large surface area of two-dimensional (2D) materials [1,2] with high conductivity with carbon quantum dots (CQDs) containing a large number of active sites is an elegant approach to achieve excellent electrode material for supercapacitor applications.

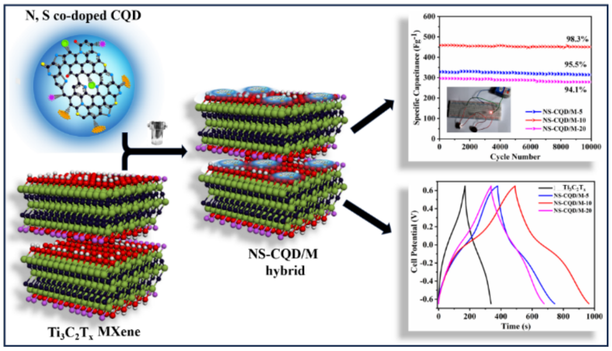

Figure 1: Graphical abstract of supercapacitive performance of NS-CQD/M hybrid

In the present work, we decorate Nitrogen, Sulfur co-doped CQDs (NS-CQDs) as source of a large number of active sites on highly conducting 2D $Ti_3C_2T_x$ MXene sheets to explore potential electrode materials for supercapacitor application [3]. We synthesize three samples exhibiting impressive specific capacitances of 562.7 Fg^{-1}, 725.7 Fg^{-1}, and 523.4 Fg^{-1} respectively at a current density of 1 Ag^{-1} with excellent cyclic stabilities of 95.5%, 98.3%, and 94.1% respectively at a current density of 10 Ag^{-1} over 10000 cycles. The origin of this high specific capacitance is the electron clouds near the 'N' and 'S' doped atoms which act as active sites. Finally, these unique hybrid composite materials with high specific capacitance, good energy density (170.34 $WhKg^{-1}$ at a power density of 1290.98 WKg^{-1}), and excellent electrochemical stability show a significant promise in the field of storage device applications.

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P-269

A Post-Synthetically Modified Cationic, Robust MOF Featuring Selective Separation of Carboxylate Containing Pharmaceutical Drugs from Water at Neutral pH: Elucidation of Adsorption Mechanism by Theory and Experiments

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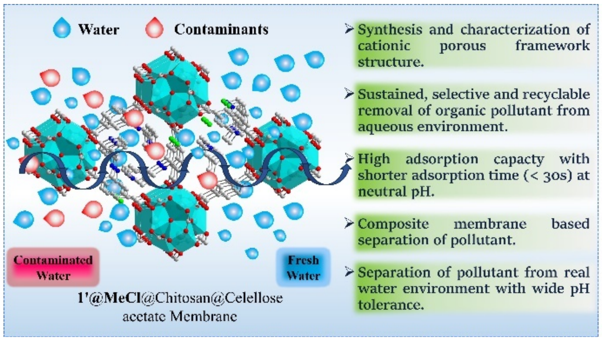
The escalating levels of hazardous pharmaceutical contaminants, specifically NSAIDs (non-steroidal anti-inflammatory drugs), in groundwater reservoir surface and surface waterways systems have prompted substantial scientific interest regarding their potential deleterious effects on both aquatic ecosystems and human health.[1,2] Extraction of those pollutants from wastewater is quite challenging. Hence, the development of economic, sustainable and scalable techniques for capturing and removing those pollutants is crucial to ensure water safety.[3] Herein, we demonstrate a physico-chemically stable, reusable, porous Hf(IV)-based cationic metal-organic framework (MOF) namely **1'@MeCl** for aqueous phase adsorption-based removal of NSAIDs (diclofenac, naproxen, ibuprofen) from wastewater environment.[4] The high positively charged surface of MOF **1'@MeCl** enables it to selectively extract more than 99% of diclofenac, naproxen, and ibuprofen contaminants within less than 30 s. With fast adsorption kinetics, very high adsorption capacities (Q_e) were achieved at neutral pH, for diclofenac (482.9 mg/g), naproxen (295.9 mg/g) and ibuprofen (219.5 mg/g). Moreover, the influence of changes in pH and co-existing anions on the adsorption property of **1'@MeCl** MOF was studied. Furthermore, the adsorption efficiency of **1'@MeCl** in different real water environments was ensured by performing diclofenac, naproxen, and ibuprofen adsorption from tap, river, and lake water. Moreover, **1'@MeCl** anchored cellulose acetate-chitosan membrane was developed successfully to demonstrate membrane-based extraction of diclofenac, naproxen, and ibuprofen from contaminated water. Furthermore, a molecular-level mechanistic study was performed through experimental and computational study to propose the plausible adsorption mechanisms for diclofenac, naproxen and ibuprofen over the surface of **1'@MeCl**.



- Synthesis and characterization of cationic porous framework structure.
- Sustained, selective and recyclable removal of organic pollutant from aqueous environment.
- High adsorption capacity with shorter adsorption time (< 30s) at neutral pH.
- Composite membrane based separation of pollutant.
- Separation of pollutant from real water environment with wide pH tolerance.

Figure 1. Graphical abstract of the cationic MOF based extraction of anionic pollutants to ensure convenient purification and supply of clean and safe drinking water for all.

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P-270

Reversible CsPbBr3 ↔ CsPb2Br5 Transformation via Reverse Micellar Aqueous Solution

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Lead-halide perovskites suffer from water and moisture instability due to the highly ionic nature of the crystal structures, though a few groups took advantage of it for the chemical transformation via water-assisted strategy. However, direct exposure of perovskite to bulk water leads to uncontrolled chemical transformation. Here, we report a controlled chemical transformation of $CsPbBr_3$ to $CsPb_2Br_5$ triggered by nanoconfined water, by placing $CsPbBr_3$ in the non-polar phase within a reverse micelle. The chemical transformation reaction is probed using steady-state and time-resolved optical spectroscopy. We observe absorption and PL in the UV region stemming clearly from the $CsPb_2Br_5$ phase upon interaction with the reverse micellar aqueous solution. Transmission electron microscopy and X-ray diffraction measurements further provide the structure and morphology. Our results direct the formation of $CsPbBr_3$-$CsPb_2Br_5$ nanocomposite under dry conditions while the chemically transformed $CsPb_2Br_5$ phase exists only in the moist condition, which we explain via the CsBr-stripping mechanism.

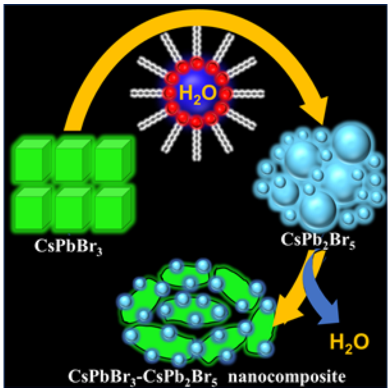

Figure.1 Graphical abstract of reversible transformation of $CsPbBr_3$↔$CsPb_2Br_5$

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P-271

LiBr-Promoted Reaction of β-Ketodithioesters and Thioamides with Sulfoxonium Ylides to Synthesize Functionalized Thiophenes

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β-ketodithioesters (b-KDTE) and β-ketothioamides (b-KTA) featuring both electrophilic and nucleophilic centers are highly versatile synthons owing to their ready accessibility and unique reactivity.[1] On the other hand, one of the significant group of reagents includes sulfoxonium ylides, which play a crucial role in facilitating numerous significant organic transformations. Sulfoxonium ylides represent a versatile and pivotal class of compounds towards organic synthesis due to their inherent advantages, such as bench-stability, easy availability and rich functional groups over the recent years.[2] The unique reactivities of these precursors make them invaluable in organic synthesis for constructing simple/complex molecular architectures. Towards our on-going interest in the strategic discovery of new methodologies *via* utilizing the exceptional features of β-ketodithioesters and derivatives, we speculated whether the sulfoxonium ylide could also react with β-ketodithioesters and thioamides to furnish significant heterocyclic scaffolds.

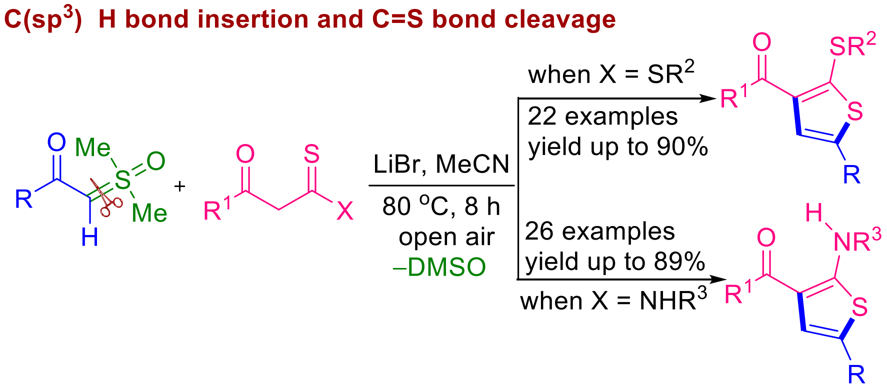

Figure 1. LiBr-promoted heteroannulation of b-KDTE/KTAs with sulfoxonium ylides

Herein, an operationally simple and highly efficient synthesis of functionalized thiophenes has been developed by Lithium bromide promoted heteroannulation of β-ketodithioesters and thioamides with bench-stable sulfoxonium ylides under mild conditions for the first time. This novel one-pot strategy involves formal Csp^3−H bond insertion and intramolecular cyclization. This approach features readily accessible starting materials, TM and additive-free condition, a broad substrate range, extensive functional group compatibility, and scalability. Moreover, the thiomethyl and carbonyl side chain in the resulting product provides a good handle for downstream transformations.

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P-272

Study of Structural Phase Transition and Optical Properties in a Series of New 0D Hybrid Metal Halides: $(3,5\text{-DMP})_2Bi_{1-x}Sb_xCl_5$

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Low-dimensional organic-inorganic metal halides (OIMHs) have garnered immense attention and extensive research in the field of solid-state lighting materials owing to their outstanding self-trapped exciton (STE)-induced luminescence properties. [1] Though there has been significant research activity in the field of lead-based hybrid metal halides, these compounds suffer from environmental toxicity and atmospheric instability. [2,3] Thus, it is significant to explore new and promising materials, containing non-toxic elements with excellent atmospheric stability and superior luminescence properties. This has led to the dawn of Bi/Sb-based OIMHs as potential substitutes for lead-based OIMHs with very good thermal and ambient stability and containing relatively less toxic and earth-abundant elements, which are crucial for large-scale commercial use. [4,5] Further, it has been observed that reduction in the dimensionality of the Bi/Sb-based OIMHs enhances their photoluminescence (PL) properties for applications in solid-state lighting devices. Moreover, understanding the relationship between the structure and luminescence properties of these materials is of utmost importance for tuning the PL properties for various practical applications.

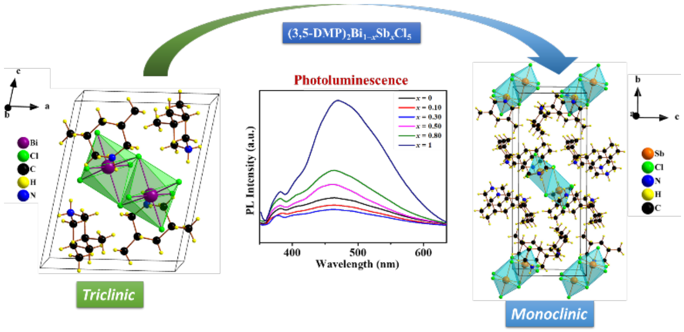

Figure 1. Graphical abstract of the structural phase transition from triclinic to monoclinic phase through Sb substitution in the series of compounds, $(3,5\text{-DMP})_2Bi_{1-x}Sb_xCl_5$ and its effect on photoluminescence properties.

To further explore the 0D lead-free hybrid metal halides, herein we report two novel organic ammonium-based 0D lead-free metal halides, $(3,5\text{-DMP})_2BiCl_5$ and $(3,5\text{-DMP})_2SbCl_5$ (3,5-DMP = 3,5-dimethylpiperidine) that crystallize in the triclinic system with $P\bar{1}$ space group and monoclinic system with $P2_1/c$ space group, respectively. The crystal structure consists of discrete isolated $[M_2Cl_{10}]^{4-}$ (M = Bi, Sb) inorganic units encased by $(3,5\text{-DMP})^+$ organic cations as confirmed by single crystal study. The structural phase transition from triclinic to monoclinic phase is further studied through the synthesis of solid solution, $(3,5\text{-DMP})_2Bi_{1-x}Sb_xCl_5$, by the substitution of Sb at Bi crystallographic site in the pristine Bi compound. The effect of the structural phase transition on the optical properties like optical band gap, PL characteristics is also studied. The compounds are further studied by various characterization techniques. [6]

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P-273

Copper-catalyzed (4+3)-cycloaddition of 4-indolylcarbinols with aziridines: stereoselective synthesis of azepinoindoles

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Copper(I)-catalyzed (4+3)-cycloaddition of 4-indolylcarbinols with aziridines has been accomplished to furnish azepinoindoles (Figure 1). The chirality transfer, substrate scope, functional group tolerance, natural product modification and tandem C-C/C-N bond formation are the important practical features.[1]

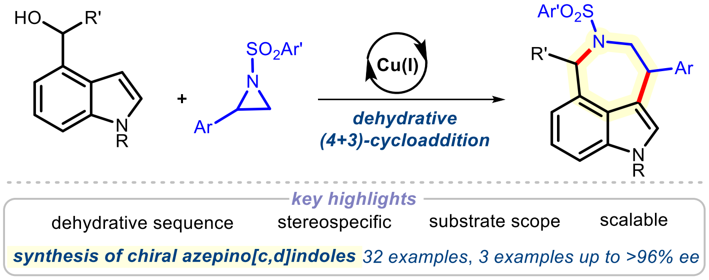

Figure 1. Dehydrative (4+3)-cycloaddition to access fused azepino[*c*, *d*]indoles.

Utilizing 4-indolylcarbinols as valuable alkylideneindoleninium ion precursors for reaction with *N*-tosyl aziridines, we herein report a stereospecific and scalable Cu(I)-catalyzed dehydrative (4+3)-cycloaddition for the generation of structurally diverse bio-relevant azepinoindoles by suppressing the undesired Mannich (3+2)-cycloadduct.

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P-274

Nanoscale Synergy: Harnessing Supramolecular Nanogel-Carbon Dots Conjugate for Enhanced Cancer Treatment through Combination Therapy

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We have designed and developed novel nanoconjugate (NG-FACD) comprises of positively charged self-assembled supramolecular nanogel (NG) derived from peptide amphiphilic hydrogelator and negatively charged folic acid functionalized blue emitting carbon dot (FACD), bound via electrostatic interactions.[1,2] Amalgamation of nanogels and carbon dots could provide promising solution by harnessing nanogels' drug delivery prowess and carbon dots' fluorescence for tracking. 'Nanogel-Carbon Dot' conjugate would emerge with enhanced cargo loading, real-time tracking and controlled drug release. Moreover, folic acid functionalized carbon dots on the surface of conjugate, enables NG-FACD to be utilized as a target-specific diagnostic probe for folate receptor-overexpressed (FR+) cancer cells and for selective cytotoxicity against (FR+) melanoma B16F10 cells over FR− lung epithelial A549 cells and noncancer HEK 293 cells by a combination of photodynamic therapy (PDT) and chemotherapy.

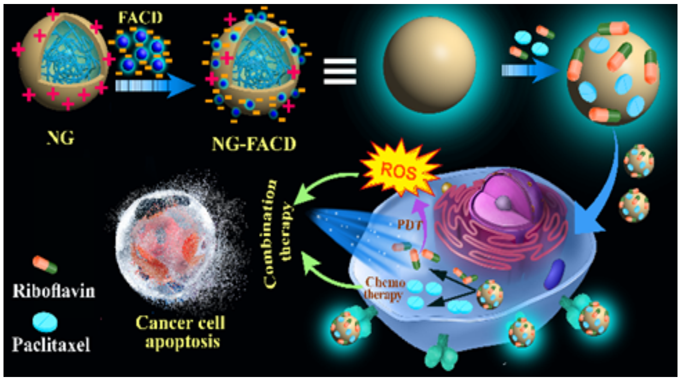

Figure 1. Nanogel-carbon dot conjugate to induce apoptosis synergistically by riboflavin mediated photodynamic therapy and paclitaxel induced chemotherapy.

Herein, we have designed novel nanogel-carbon dot conjugate (NG-FACD) for targeted delivery of a photosensitizer (riboflavin (RbF)) and a drug (Paclitaxel (PTX) for synergistic photodynamic and chemotherapy. The dual strategy, i.e., binding of paclitaxel to microtubules and ROS-mediated chromosome breakage, helps to kill malignant cells through inhibition of cell replication and migration. NG-FACD demonstrated improved riboflavin (RbF) and paclitaxel (PTX) loading compared to individual nanocarriers that made it ~1.8- and 1.5-fold higher cytotoxic towards FR+ B16F10 cells over RbF and PTX loaded individual nanocarrier (Figure 1). The concurrent presence of RbF and PTX on NG-FACD displayed ~1.9-2.8-fold higher cytotoxicity than single drug loaded individual nanocarrier and ~3-4.5-fold higher cytotoxicity through RbF mediated photodynamic and PTX induced chemotherapy in synergism compared to free drug against FR+ B16F10 cells.[3]

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P-275

Sulfur-tuned MoS_2 quantum dot decorated $Ti_3C_2T_x$ (MXene) electrode materials for high performance supercapacitor applications

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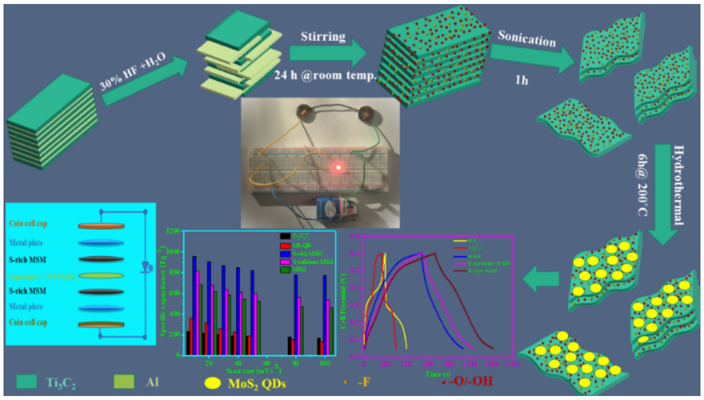
Recently, two dimensional materials have been considered as the exciting and most promising materials in the field of energy storage applications. Literature results show that the non-bridging 'S' in MoS_2 quantum dot act as efficient active sites for catalytic activity. But, the MoS_2 quantum dots with sufficient non-bridging sulfur do not possess high electronic conductivity which is required for supercapacitor electrode applications. Therefore, exploiting large number of active sites and superior electronic conductivity in the present work we have decorated $Ti_3C_2T_x$ sheets by MoS_2 quantum dots with a large number of non-bridging 'S'. We have synthesized three composite samples by varying 'S' components and seen that the sulfur rich samples show the highest value of specific capacitance (SC) of about 985 Fg^{-1} because of the presence of unsaturated sulfur S_2^{2-}ligands. The unique combination of MoS_2 quantum dot and $Ti_3C_2T_x$ shows excellent performance over a wide range of potential windows (-0.3/0.4 V to -0.7/0.8 V) with a high energy density 165.53 $WhKg^{-1}$ at a power density 1100 WKg^{-1}. Also, the SC retention values after 10^4 cycles are obtained over 96.53 % at a current density (CD) 10 Ag^{-1}.



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P-276

The *Z*-enoate assisted Meyer-Schuster rearrangement (MSR) as a tool for the construction of vinyl sulfides

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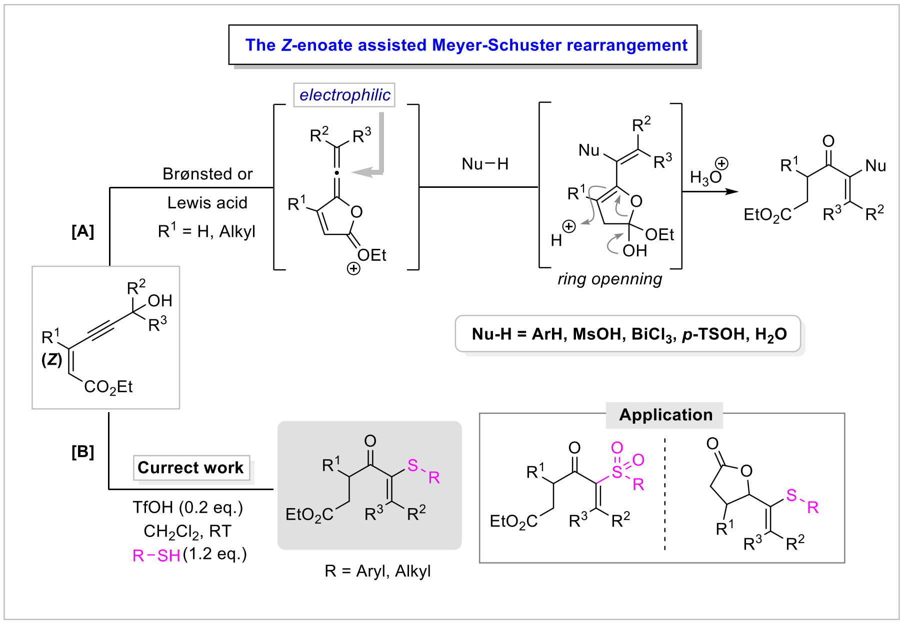
In 2016, our research group developed a new variant of the classical Meyer–Schuster rearrangement (MSR): the *Z*-enoate assisted (nucleophile intercepted) Meyer-Schuster rearrangement, which gives α, β-enones, and α-functionalized enones respectively. As part of the exploratory studies of this strategy, various nucleophiles such as Ar-H, *hetero*-arenes, $^-$OMs, $^-$OTs, Cl^-, and H_2O have already been employed as nucleophiles providing access to 1,4-ketoesters, 1,2-diketones, polycyclic enones.[1] In continuation to this, we planned to employ thiols as external nucleophiles for the rapid generation of important functional groups, the vinyl sulfides. Vinyl sulfides are extensively used as valuable synthons for enolate and acyl anions·[2,3] In addition to small molecule synthesis, vinyl sulfides are crucial building blocks in producing sulfur-containing polymers [4] as well as have applications in advanced optoelectronic materials. [5] The poster details the design and development of this methodology.



Scheme: **[A]** *Z*-enoate assisted, nucleophile intercepted M–S rearrangement. **[B]** Construction of functionalized vinyl sulfide using *Z*-enoate MSR

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Application of Crystal Engineering in the Dimerization of C=N Bond

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The reactions in the solid state offer a unique opportunity to synthesize complex molecules with wonderful regio- and stereo-specificity compared to conventional organic synthetic methodologies.[1] From the perspective of crystal engineering, [2+2] photocyclodimerization in the crystalline state has been investigated widely in the past few decades.[2] The innovative work of Schmidt, which described a “topochemical principle” for solid-state [2+2] photoreactions; states that a pair of double bonds must be aligned parallel and the distance between them should be less than 4.2 Å.[3] This principle led to the conclusion that the photodimerization proceeded with minimum atomic movement and was used to account for head-to-head and head-to-tail dimers formed upon irradiation by ultraviolet-(UV) light.[4] By utilizing the ‘topochemical principle’ extensive studies have been done on the C=C bond photodimerization, but a few reports have been published on the C=N bond photodimerization. This may be due to the low reactivity of the C=N group or low stability of the resulting diazetidines.[5] We are interested in utilizing the topochemical principle and studying the possible dimerization of the C=N bond using simple aromatic compounds. Our results will be highlighted in the poster presentation.

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P-278

Sustainable Fabrication of WO_3 Nanodices for Enhanced Ciprofloxacin Degradation

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Contaminated water poses serious risks to human health and the environment, with traditional treatment methods often falling short. Photocatalysis, however, offers a promising solution by breaking down organic pollutants using light.[1] Recent advancements focus on nanostructured photocatalysts, especially those activated by visible light, due to their efficient sunlight utilization and low energy requirements.[2]

Enhancing these photocatalysts' performance involves strategies like phase control, surface sensitization, and doping.[3] One challenge is the high recombination rate of photo-generated electron-hole pairs, which can be addressed by integrating carbonaceous materials, such as activated carbon (AC). AC's high surface area and pore structure enable effective adsorption of pollutants and facilitate reactions that reduce electron-hole recombination.[4]

We are currently investigating the developmentof composites with metal oxides using activated carbon (AC). The inclusion of carbonaceous materials facilitates the reaction between adsorbed oxygen and photogenerated electrons, effectively reducing the recombination of electron-hole pairs.This combination promotes efficient adsorption and photocatalytic oxidation due to AC’s functional groups, which help prevent recombination as well release of toxic by-products.

In summary, integrating AC with metal oxides shows significant potential for creating efficient, sustainable photocatalysts for water treatment, addressing both environmental and economic concerns.

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P-279

Non-template Synthesis of Furo[2,3-*b*]pyrrolo[2,3-*d*]pyridines via Pd(II)-Catalyzed Dual N−H/C Annulative-Cyclization

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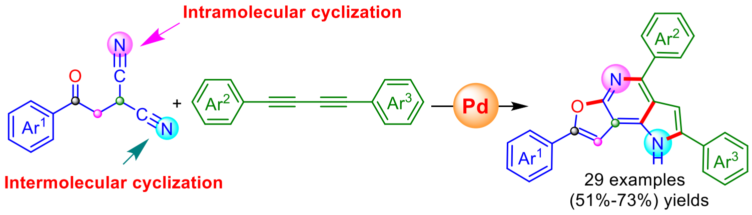
A Pd(II)-catalyzed non-template synthesis of furo[2,3-*b*]pyrrolo[2,3-*d*]pyridines from b-ketodinitriles and diynes has been accomplished via dual annulative cyclization. The participation of both the nitrile (-CN) groups led to the concurrent construction of three heterocycles *viz.* furan, pyrrole, and pyridine forming C-C, C=C, C-O, C-N, and C=N bonds. The synthetic utility of the protocol was further demonstrated through a few post-synthetic manipulations.



- concurrent formation of furan, pyridine and pyrrole
- participation of both −CN groups
- formation of C–C, C=C, C–O, C–N, and C=N bonds
- non-template synthesis of furo-pyrrolo-pyridines
- double N–H/C annulative cyclization
- easily accessible precursors
- post-synthetic functionalizations

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P-280

Argentophilic Interaction in 6-chloro-7-methylpurine: Role of Anions in Structural, Electrical and Ionic Properties

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Artificial neural networks rely heavily on on-chip memory to minimize data transfer between memory and the processor, thereby efficiently handling complex algorithms and large datasets.[1] Metal Organic Frameworks (MOFs) are now being used to make memory storage devices. Generally, MOFs are non-conductive in nature. However suitable structural modulation can make MOFs semi-conductive/ conductive. To exhibit artificial neural network like behaviour, MOFs must possess both electronic and ionic conductivity.[2] Purine nucleobases, such as adenine and its derivatives, are studied extensively for their interaction with metal ions.[3] We have synthesised and characterized a series of N7-alkylated purine-based MOFs incorporating Ag^+ ions, finding that variation in anions show improved conducting properties. Our findings demonstrates that non-coordinating anions ($BF_4^- < PF_6^- < SbF_6^-$) exhibit greater mobility and conductivity under an applied voltage bias, whereas the oxygen coordination in nitrate restricts its movement, resulting in minimal conductivity. Consequently, MOFs with a combination of both types of anions display intermediate conductivity, highlighting the potential for tuning anion composition to optimize the conductivity of MOFs.

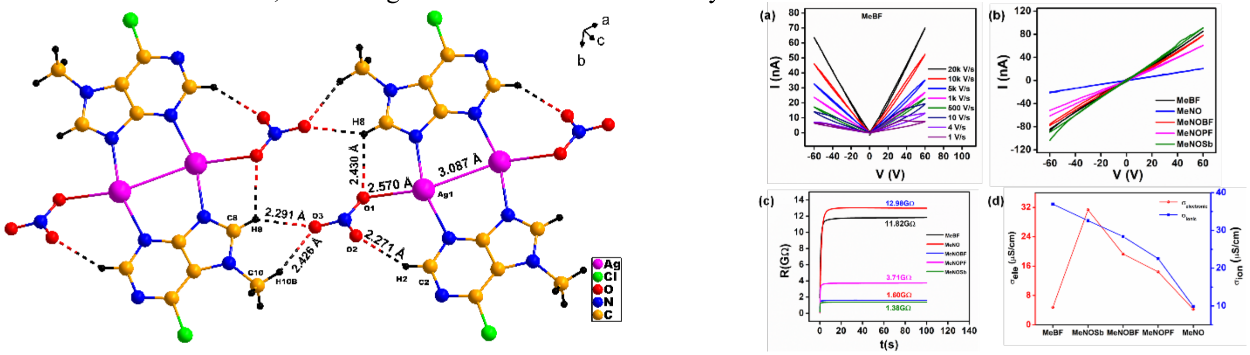

Figure 1. Crystal Structure of silver-purine MOF and its conductivity with varying anions.

This poster presents diverse coordination geometries around the silver ion, as well as conductivity of MOFs having different anions. We also conducted molecular docking studies with various protein residues from cancerous cells as silver is well known for its antibacterial, antiviral and anticancer property. Molecular Docking study shows $MCPNO_3$ exhibited highly promising results, highlighting its potential for further biological applications.

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P-281

Synthesis of SMAC mimetics for the treatment of cancer

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SMAC mimetics are small-molecule entities that mimic the activity of the second mitochondria-derived activator of caspases (SMAC) protein, targeting inhibitors of apoptosis (IAP) proteins to suppress their function and facilitate apoptosis. [1] With its IAP-binding motifs (IBM), SMAC interacts with the BIR2 and BIR3 domains of IAPs to inhibit its functions. The IBM domain consists of four amino acid residues (AVPI) and prevents the interaction of XIAP with caspase-3, caspase-7, and caspase-9. Having the structural importance of the AVPI domain for the interaction of SMAC with XIAP, several NCEs (LCL-161, Birinapant, AT-406, ASTEX-660) were designed that mimic the secondary structure AVPI and few of them have shown good progress in clinical trials.[2]

Herein, we have prepared various C5-substituted unnatural proline-based amino acids. Incorporating these amino acids into the AVPI unit showed good bioactivity against the breast cancer cell lines.

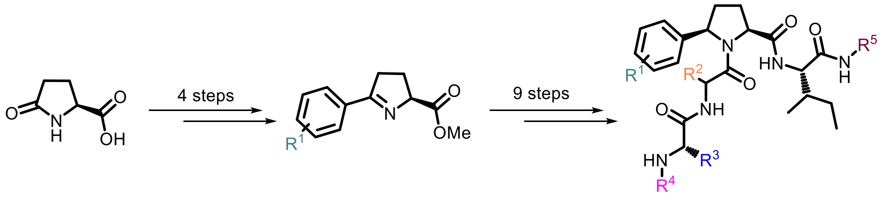

Figure 1: Synthesis of proline-based unnatural amino acid and its incorporation in SMAC mimetics

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P-282

Pharmacophore-based Dual-target Drug Profiling for Alzheimer's Disease

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Alzheimer's disease is characterized by amyloid plaques, neurofibrillary tangles, and finally neurodegeneration. It's a neurodegenerative disease and most aged people suffer from this disease. According to the Amyloid hypothesis, in the amyloidogenic pathway, APP (Amyloid Precursor Protein) is first cleaved by the β-secretase (BACE1) enzyme into sAPPβ and CTF99, and this CTF99 is further cleaved by γ-secretase into Aβ and AICD. Also according to Tau hypotheses, tau protein is hyperphosphorylated and it depolymerizes microtubules and affects signal transmission. This hyperphosphorylation of tau protein is due to increased GSK3β activity. Overactivity of BACE1 & GSK3β is one of the reasons for cognitive dysfunction in Alzheimer's disease. In recent times research on dual-target drugs is going on to find molecules that can inhibit both proteins [1]. There are several drugs in the market but these medications often come with some side effects. That's why an effective drug is required for Alzheimer's disease to overcome those side effects.

In this work, our goal is to find drug molecules that can inhibit both proteins effectively with good ADME properties. At first, 10 preestablished compounds for each protein i.e. for BACE1 & GSK3β were taken from the PubChem database to generate their common pharmacophore features [2]. After that, the database of 4848 molecules, taken from the NCI (National Cancer Institute) database was mapped into the generated pharmacophores to see how well they fit into that. We have considered those molecules having more than 60% fit value of the best-fit value of the molecules used to generate pharmacophores. Additionally, molecular docking [3] of those molecules has been performed with both the target proteins i.e. BACE1 (PDB ID- 4J0P) & GSK3β (PDB ID- 1PYX). Finally, we have shortlisted one molecule out of those, showing a better docking efficiency with both the target protein and excellent ADME properties which are required for the effective treatment of Alzheimer's disease. Following this methodology we have shortlisted one molecule out of 35 molecules that satisfies all crucial parameters and shows better molecular interactions with the amino acid residues of the proteins. So, it might be a promising drug molecule after successful preclinical and clinical trials.

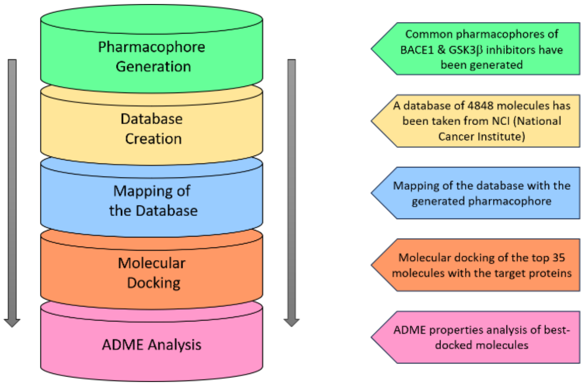

Figure 1. Graphical abstract of the Methodology for pharmacophore-based drug profiling for Alzheimer's Disease

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P-283

Synthesis of Thioamide Derivatives in Environmentally Benign Deep Eutectic Solvent (DES): A Green Approach

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Deep Eutectic Solvents (DESs) have gained increasing attention over the past few years in various organic synthesis due to their green solvent properties and potential to enhance the reaction rates and selectivity. DES has some unique properties like low toxicity and biodegradability, high tunability and solvating ability, and easy preparation method.[1] Willgerodt-Kindler (WK) reaction [2] is one of the most popular methods for Thioamide synthesis. These thioamide compounds are widely used for the synthesis of different pharmaceutical drugs, bioactive compounds and functional materials. In this presentation, we have discussed a mild, efficient, simple, and greener approach towards a series of thioamide derivatives synthesis following the WK reaction in a metal-free choline chloride (ChCl)-urea (1:2) DES.[3]

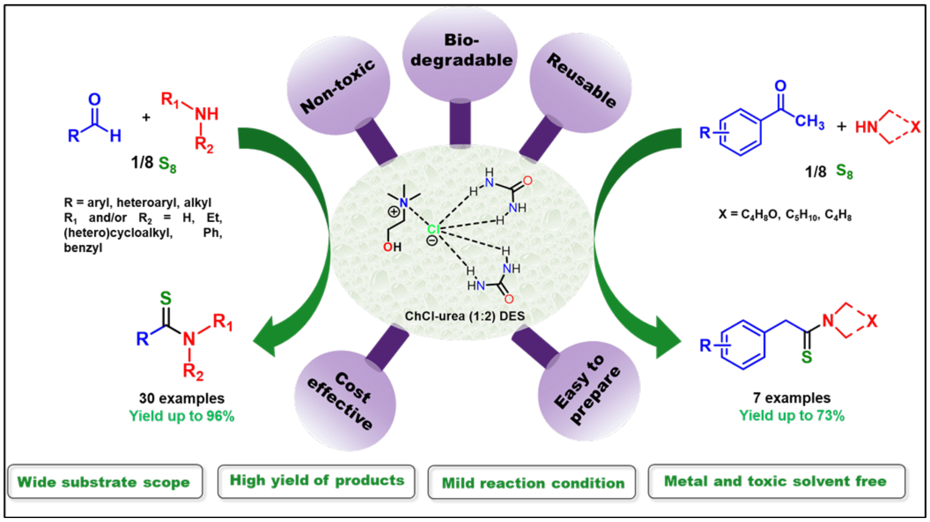

Figure 1. Graphical abstract of thioamide synthesis in ChCl-urea (1:2) DES

Here we have synthesized a wide variety of thioamide derivatives in good-to-excellent yields by the reaction of different substituted aldehydes/ketones, secondary amines, and elemental sulfur in ChCl-urea (1:2)–based deep eutectic solvent (DES). Further, we have utilized our prepared thioamides for the synthesis of thiadiazole derivatives. We have performed gram-scale reactions also to show the industrial scalability of this methodology. Our protocol significantly enhances sustainability (i) as the reaction is performed at low temperature so less energy consumption and (ii) less waste generation as the stoichiometric amount of reactants are used. Here DES is only used as a green solvent as well as a non-toxic catalyst without the addition of any other catalyst or solvent and this DES can be recycled and reused several times without any significant loss of its activity.

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P-284

Selective Sensing of L-Cysteine by Silver Nanogranules Incorporated RhB Nanocomposites

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Amino acid sensing is a cutting-edge research area for early illness detection and monitoring. Among the numerous amino acids, L-Cysteine (L-Cys) sensing is critical for the identification of human disorders such as neurotoxic impact and coronary heart disease, which are caused by an excess of L-Cys. To address this, we present a relatively simple way of L-Cys sensing using a fluorescence "TURN ON" mechanism involving silver-centred Rhodamine B nanogranules (AgNPs/RhB). The as-synthesized nanocomposite fluorescent probe exhibits very selective sensitivity towards L-Cys, assisted by the preferential and stable covalent linkages between AgNPs and the thiol group of L-Cys, as validated by FTIR and XPS studies. The study adds to the current literature by demonstrating improved selectivity of L-Cys in the presence of other amino acids and interacting ions. It has a limit of detection (LOD) of 1.084 µM and a working linear range of 100-2200 µM. The nanogranules' capacity to respond to extreme ionic strength and pH conditions adds to their stability and applicability for the current application. Furthermore, the high recovery percentages reported in real human serum samples demonstrate its utility in diagnostic applications.

Keywords: *L-Cysteine; Silver; Rhodamine B; Sensing; Nanogranules; Fluorescence*

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P-285

Pyridine-bridged Molecular Flexibility and its impact on FWHM and ΔE_{ST}

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We have designed a rigid emitter, CzPyFO and the flexible emitter, CzPyPB. Herein, by keeping the pyridine bridge between the donor and an acceptor moiety we aim to improve the dihedral angle and oscillator strength[1]. The rigid emitter shows a cyan-blue emission with the full width half maxima (FWHM) of 83 nm and singlet-triplet energy gap (ΔE_{ST}) of 0.08 eV. In contrast, on introducing flexibility, the FWHM of the emitter decreases to 33 nm, which deviates from the conventional trend and the ΔE_{ST} increases significantly to 0.5 eV. Thus, there is a notable change in FWHM just by breaking the bond. A strong electron-accepting group can be incorporated into the flexible molecular structure to further lower the ΔE_{ST} without greatly affecting on the FWHM and the emission maxima. The molecule with strong electron accepting group can be further used for sensing purposes[2].

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P-286

Redox-neutral zinc-catalyzed cascade [1,4]-H shift/annulation of diaziridines with donor-acceptor aziridines

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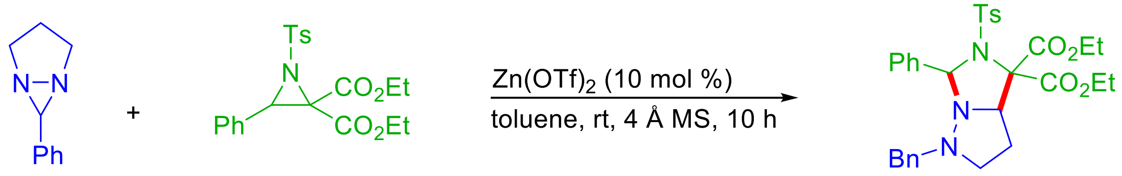
Expeditious access to Imidazopyrazole scaffold *via* 1,4-Hydride shift triggered C(*sp3*)-H bond functionalization/ cyclization of diaziridines[1] with donor-acceptor aziridines[2] has been developed in presence of Zn-catalyst. The *in situ* generated pyrazoline intermediate was successfully isolated to unveil the unusual (2+n) reactivity of diaziridine.[3] Notably, this methodology facile to construct the corresponding fused heterocycles from moderate to good yields and can be easily expanded to gram scale under mild condition. In addition, natural product mutation and a late stage *in silico* molecular docking study to showcase antifungal activity are the significant features.



✓ Broad substrate scope

✓ Fused heterocycles

✓ Mild reaction conditions

✓ Molecular docking study

Figure 1. Zn-catalyzed (3+2)-annulation of diaziridine with donor-acceptor aziridine

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P-287

Diorganotin(IV) complexes with bulky quadridentate salphen-type Schiff base (N_2O_2) incorporating diazenylpyridyl side arms

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Schiff bases are considered as privileged ligands due to their modular synthesis, allowing control of the nature of donor atoms, denticity, chelating ability, as well as electronic and steric properties [1]. Plentiful metal complexes of ter- and quadri-dentate Schiff-base ligands have been investigated owing to their distinctive and manifold physico-chemical, structural properties and catalytic activity, well documented in recent literature [2]. Applications of Schiff-base metal complexes with high denticity and prominent functional properties are also available [3]. We shall confine our discussion solely to a class of N_2O_2 quadridentate bis-Schiff base such as salphen.

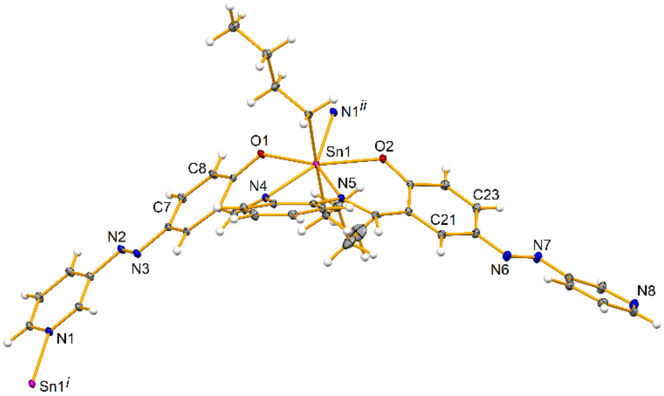

Figure. 1. Ellipsoid plot of *n*-Bu_2SnL (**1**) with partial atom labeling schemes.

Tetradentate-N_2O_2 ligand (H_2L) was generated by imine condensation of one equivalent of benzene-1,2-diamine with two equivalents of 2-hydroxy-5-(pyridin-3-yldiazenyl)benzaldehyde. Subsequently, two new diorganotin(IV) complexes of composition R_2SnL [R = *n*-Bu (**1**), Ph (**2**)] were accomplished from the reactions of H_2L with diorganotin oxides in refluxing toluene. Complexes have been characterized by IR, multinuclear NMR (^1H, ^{13}C and ^{119}Sn) spectroscopy.^{119}Sn spectroscopy confirmed that the complexes **1**-**2** are six-coordinate in solution. X-ray diffraction studies showed the Sn(IV) center is six coordinated surrounded by the κ-O^2N^2 tetra-dentate chelating ligand and two Sn-R ligand. Polymeric structure of the compound *n*-Bu_2SnL (**1**) is generated through the pendent pyridine nitrogen atom. Although solid state crystallographic results revealed asymmetrical molecular configurations, solution NMR studies indicated that the compounds exhibit symmetrical structures in solution. More results will be discussed.

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P-288

Synthesis, characterization and study of catalytic degradation of methyl orange by an oxidovanadium(IV) Schiff base complex derived from glycine

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Environmental concerns are raised worldwide by the discharge of wastewaters from the textile industry that contain organic contaminants [1, 2]. Azo dyes, the largest group of synthetic pigments makes up more than 50% of all commercial dyes are extensively employed by the textile industries [3]. Vanadium complexes have shown potential as active catalysts for oxidation of organic substrates in presence of suitable oxidants like H_2O_2, where the vanadium^{+} ion interacts with H_2O_2 in Fenton-type reactions to form hydroxyl radicals [4].

A Schiff base oxidovanadium complex derived from glycine and salicylaldehyde with phenanthroline as co-ligand *viz.*[VO(salgly)(phen)].4H_2O (**1**)(where salgly = Schiff base derived from salicylaldehyde and glycine, phen = 1,10-phenanthroline) was synthesized under ambient conditions. The complex was characterized by elemental analysis and spectroscopic techniques such as FT-IR, UV-Vis and electron paramagnetic resonance (EPR). The structure of the complex was determined by single crystal X-ray diffraction. The crystal packing of **1** is stabilized by π···π stacking and C-H···O hydrogen bonding interactions. Moreover, the harmful azo dye, methyl orange, which is used extensively in textile industries, has been selected as a model contaminant [5, 6]. The degradation of methyl orange dye by the title complex in presence and in absence of hydrogen peroxidewas investigated. The result shows that the complex **1** has good catalytic activity towards degradation of methyl orange in presence of hydrogen peroxide.

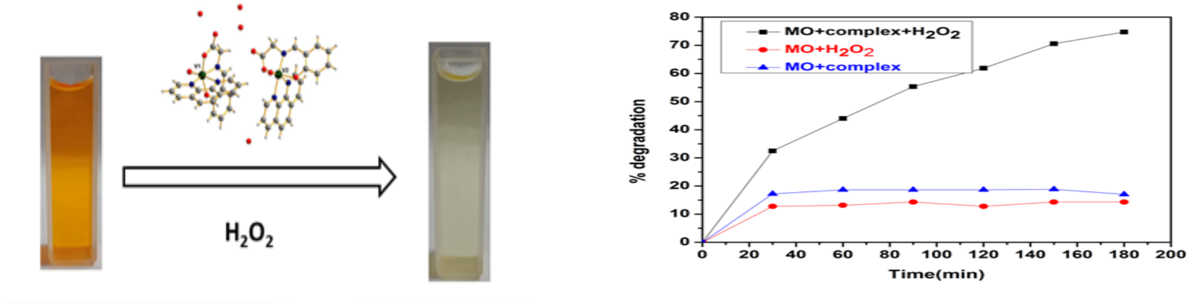

Figure 1: Catalytic Degradation of Methyl Orange by [VO(salgly)(phen)].4H_2O (**1**) in presence of H_2O_2

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P-289

One-pot facile green synthesis of ruthenium nanoparticles embedded in the nanoglobules of aloevera gel with anticancer potential

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Metal nanoparticles have a noteworthy future in cancer treatment research because of their smaller size and large active surface area. Though gold, silver, platinum, palladium, copper, zinc, iron and several other metal nanoparticles have been explored for their anticancer potential in different pathways, the main limitation of these particles is their toxicity which may be controlled through their size, surface modification and route of administration [1-3]. Compared to other metal nanoparticles, ruthenium nanoparticles have high bio compatibility and they exhibit excellent photo-thermal effect. Though there are several reports in the literature on the anticancer potential of ruthenium complexes, ruthenium nanoparticles are not much investigated [4]. In the present work, therefore, an attempt has been made to synthesize ruthenium nanoparticles in an easy and eco-friendly way using Aloe vera gel. Ruthenium chloride was used as a precursor and Aloe vera gel acted both as reducing and capping agent. The synthesized ruthenium nanoparticles were characterized using UV-Visible spectrophotometry, Fourier Transform Infrared Spectroscopy (FT-IR), High Resolution Transmission Electron Microscopy (HRTEM), Powder X-ray Diffraction (PXRD), Dynamic Light Scattering (DLS) and Field Emission Scanning Electron Microscopy (FESEM). The analyses confirmed the formation of nano globules of Aloe vera gel of diameter in the range 90–300 nm with ruthenium nanoparticles of average size 1.5 nm embedded in them. The synthesized Ru nanoparticles embedded in the nano globules of Aloe vera gel (ALV RuNPs) were explored for their anticancer potential in the Dalton's lymphoma ascites (DL) cell line using Trypan Blue assay. The results of the assay showed that the ALV RuNPs can induce concentration dependent cytotoxicity in DL cancer cells. Approximately 40 % cytotoxicity was obtained for concentration range 5–50 mg/mL of the sample while negligible cytotoxicity was observed for healthy PBMC cells. The results showed that ruthenium nanoparticles can emerge as a promising bio-compatible candidate with the ability to selectively target cancer cells while sparing normal cells.

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P-290

Point-of-Care Testing of Uric Acid Using Gold Nanostar Embedded Robust and Reusable Hydrogel Beads Showing Photo-Oxidase Like Activity

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A system is presented here that capitalizes on the unique photo-oxidase-like activity of gold-nanostars, which are embedded onto the surface of hydrogel beads, to achieve highly sensitive and precise uric acid detection. In contrast to conventional gold-based nanocatalysts, these gold-nanostars demonstrate specific oxidase-like activity when exposed to light. [1] Integrating the gold nanostars onto the hydrogel bead surface mitigates the problem of catalytic activity loss due to agglomeration, thereby significantly enhancing the catalytic stability. [2] This enhancement is demonstrated by the sustained catalytic activity, even after prolonged incubation in aqueous medium for 60 days. Moreover, the beads exhibit robust performance over multiple cycles. The mechanism of uric acid sensing involves the oxidation of chromogenic substrate TMB by the embedded gold nanostars, followed by reduction of oxidized TMB upon interaction with uric acid, resulting in a noticeable color change. This color change can be quantitatively analyzed to determine the levels of uric acid with a remarkable detection limit of 0.9 µM. The integration of smartphone technology enabled swift and convenient on-site testing, bridging the gap between laboratory settings and real-world applications. This is further supported by the system's excellent accuracy in analyzing blood serum as well as urine samples.

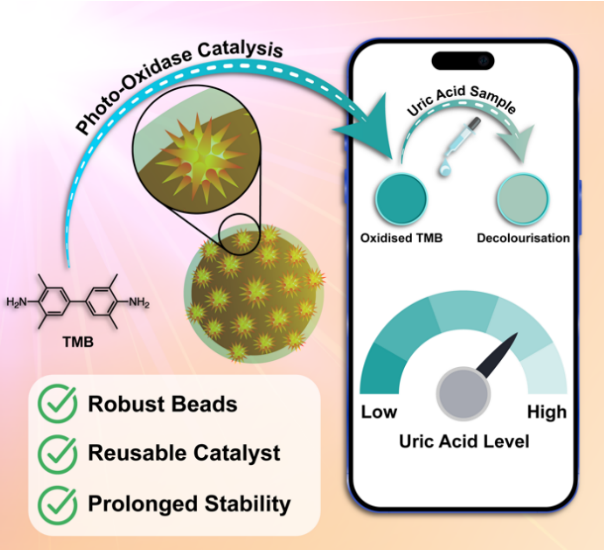

Figure 1: Graphical representation of uric acid detection via photo-oxidase catalysis

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P-291

Blossoms of Health: A Review of the Nutraceutical and Medicinal Properties of Indian Flowers

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Indian flowers have been known for their medicinal and nutraceutical properties, deeply rooted in traditional healing systems like Ayurveda, Unani, Siddha, and Homeopathy. This review explores the nutritional value, chemical composition, and therapeutic potential of various Indian flowers, highlighting their diverse applications in promoting health and well-being.[1]

Flowers such as hibiscus (*Hibiscus rosa-sinensis*), marigold (*Tagetes erecta*), lotus (*Nelumbo nucifera*), and rose (*Rosa rubiginosa*) contain a variety of bioactive compounds, including flavonoids, alkaloids, phenolic acids, tannins, and essential oils, which contribute to their therapeutic efficacy. For instance, hibiscus is rich in anthocyanins, which possess potent antioxidant and anti-inflammatory properties, while marigold contains carotenoids that promote skin health and wound healings.[2]

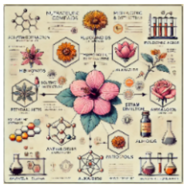

Figure 1. Graphical abstract

The extraction methods for isolating these bioactive compounds vary from simple aqueous or ethanol extraction to advanced techniques like supercritical fluid extraction and ultrasound-assisted extraction.[3] These methods help preserve the flowers' nutritional components, ensuring that key compounds such as vitamins (A, C, and E), minerals, and essential amino acids are retained.

Ayurveda considers many Indian flowers as balancing agents for the body’s doshas (Vata, Pitta, Kapha), with applications in treating ailments ranging from digestive disorders to skin problems. Similarly, the Unani and Siddha systems use flower-based formulations for their cooling, anti-inflammatory, and rejuvenating effects. Homeopathy taps into the subtle healing potential of flower essences to restore emotional and mental balance.[4]

In conclusion, the medicinal and nutraceutical value of Indian flowers is rooted in their rich phytochemical profile and cultural heritage. Future research should focus on making them more accessible for modern healthcare applications.

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P-292

Selective sequential oxidation of *N*-substituted tetrahydroquinoline using cyclometalated ruthenium(II) complex

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α-methylene oxidation of structurally diverse *N*-substituted tetrahydroquinolines to lactams has been developed using cyclometalated Ru(II)-complex as a catalyst.[1] Cyclic-α-methylene C–H bonds were selectively oxidized in the presence of *α*-methyl or reactive α-methylene C–H bonds. This methodology has been successfully utilized in the late-stage functionalization and diversification of pharmaceuticals. The reaction pathway involves Ru(VI)-dioxo species as one of the key intermediate that has been spectroscopically characterized. In the given case, high valent metal-oxo species might be stabilized by strong s-donation and p-delocalisation from the ligand with annulated backbone. Along with notable selectivity, control over selective oxidation of active sites has been observed by varying the equivalency of oxidant ($NaIO_4$) and catalyst loading. Furthermore, protocol allows selective sequential functionalization of complex molecules. Sulfur-functionalized compound gives corresponding sulfoxide and sulfone. Further, terminal alkyne is oxidised to give terminal acid.

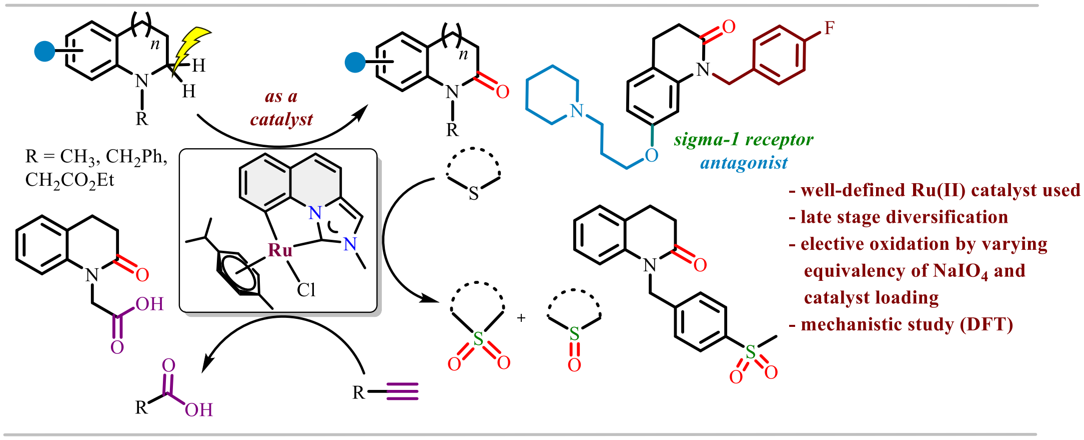

Figure 1. Graphical abstract of selective sequential oxidation of *N*-substituted tetrahydroquinolines

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P-293

Synthesis of 1,2,3,4-Tetrahydroquinolines from *N*-Unsubstituted Aminomethyl Donor-Acceptor Cyclopropanes

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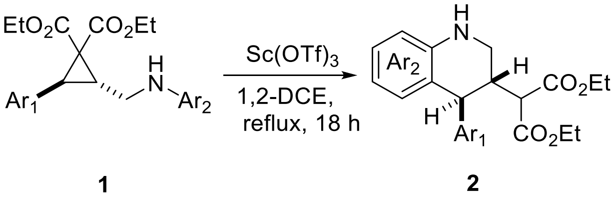
Tetrahydroquinoline is an important heterocyclic motif found in numerous natural products and pharmaceutically active compounds.[1] Given the importance of tetrahydroquinolines, it is not surprising to note that a large number of methods have been reported for the synthesis of tetrahydroquinolines.[2] Donor-acceptor cyclopropanes (DACs) are one of the versatile building blocks in organic synthesis for accessing heterocyclic compounds.[3] We have recently reported that aminomethyl-substituted DACs, when treated with a catalytic amount of $Yb(OTf)_3$ in 1,2-DCE afforded tetrahydroquinolines though intramolecular arylative ring-opening.[4] During the course of the investigation, we noticed that when *N*-unsubstituted DACs were used in the study, the reaction did not take place, probably due to strong coordination of the Lewis acid to nitrogen. So, in the present study, we employed Sc $(OTf)_3$ as the Lewis acid for the transformation and successfully obtained a series of tetrahydroquinolines **2** in good yields from *N*-unsubstituted aminomethyl cyclopropanes **1** (Scheme 1). The details will be presented in the poster.



Scheme 1

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P-294

Green synthesis of Schiff base containing sulphur bond and its Cu(II) complexes: Crystal structure Analysis, Hirshfield Analysis, DNA binding studies, in-vitro biological Assessment, quantum chemical calculations and Docking studies.

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Abstract: A novel Schiff base, L was successfully synthesized through heatless condensation between 2,2'-diaminodiphenyl disulfide and o-vanillin. The structure of the synthesized Schiff base was confirmed by single-crystal X-ray diffraction analysis, which provided precise details on the molecular geometry. Further structural insights were obtained using Hirshfeld surface analysis, revealing the presence of significant intermolecular interactions between the ligand molecules, which contribute to the stability of the crystal packing[1]. Subsequently, three copper(II) complexes, LCu1, LCu2, and LCu3, were synthesized using ultrasonic irradiation as a green, energy-efficient method[2]. Comprehensive characterization of the synthesized complexes was carried out using various analytical techniques, including elemental analysis, FTIR spectroscopy, UV-Vis spectroscopy, EPR spectroscopy, mass spectrometry, and Job's method of continuous variation. Quantum Chemical calculations further validated the structural and stability aspects of these complexes, establishing a stability order of LCu1 < LCu3 < LCu2 < L. DNA binding properties of the copper complexes were extensively studied using UV-Vis spectroscopy, fluorescence quenching assays, and viscosity measurements. These studies confirmed that the complexes exhibit intercalative binding with DNA, with intrinsic binding constants (K_b) and quenching constants (K_{sv}) values of the order of 10^5 M^{-1}. Among the synthesized complexes, LCu3 demonstrated the strongest interaction with DNA and also exhibited the highest antibacterial activity, particularly against gram-positive bacteria, with a zone of inhibition reaching up to 13 mm. It also showed the lowest minimum inhibitory concentration (MIC) values, indicating its potent antibacterial efficacy. In addition to its antimicrobial properties, LCu3 was found to possess significant antioxidant and anti-inflammatory activities. These biological activities were evaluated using the DPPH free radical scavenging assay for antioxidant potential and the Egg albumin denaturation assay for anti-inflammatory effects. Molecular docking studies further supported these findings, with the complexes showing strong binding affinities towards CT-DNA. The synthesized Schiff base and its copper complexes, particularly LCu3, demonstrate promising potential for use in medicinal chemistry and biological studies, highlighting their versatility in drug development and therapeutic interventions.

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P-295

Facile Fabrication of multi-functional super hydrophobic surfaces synthesized by additive manufacturing technique modified with ZnO nanoparticles

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This article reports facile fabrication of a multi-functional smart surface having super-hydrophobic self-cleaning property, super-oleophilicity and anti-microbial property. These smart surfaces have been synthesized using the stereolithography method of the additive manufacturing technique. Stereolithography is a fast additive manufacturing technique used to create complex parts with intricate geometries. A wide variety of materials and high-resolution techniques can be utilized to create functional parts, such as superhydrophobic surfaces. Various materials have been studied to improve the functionality of 3D printing. However, the fabrication of such materials is not easy as it is quite expensive. In this work, we used a commercially available SLA printer and its photopolymer resin to create various micro-patterned surfaces. Additionally, we applied a low surface energy coating with ZnO nanoparticles and Tetraethyl orthosilicate (TEOS) to create hierarchical roughness. The wettability studies of created superhydrophobic surfaces were evaluated by means of static contact angle using sessile drop method and rolling angle measurements. The effects of various factors, including different concentrations of coating mixture, drying temperatures, patterns (pyramids, pillars, and eggbeater structures), and pillar spacing, were studied in relation to contact angles. Subsequently, all the functional properties (i.e., self-cleaning, oleophilicity, anti-bacterial properties) of the as-obtained surfaces were demonstrated using data, images and supporting videos. This inexpensive and scalable process can be easily replicated with an SLA 3D printer and photopolymer resin for many applications such as self-cleaning, oil-water separation, channel- less microfluidics, anti-bacterial coating etc.

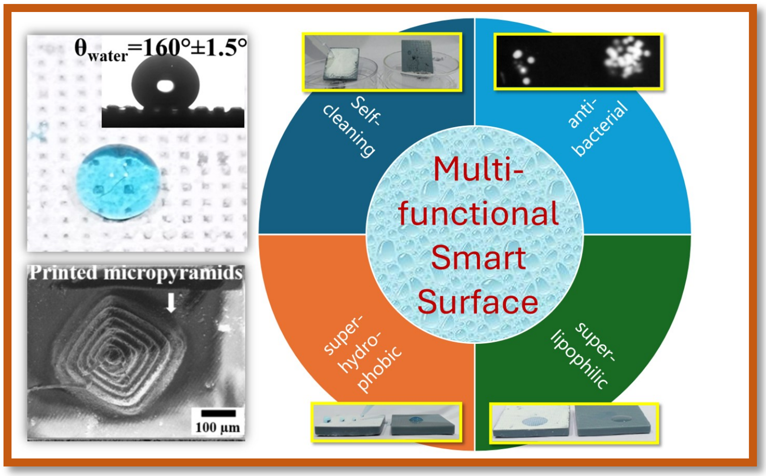

Figure 1. Graphical abstract of the multi-functional superhydrophobic surface

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P-296

GC-MS analysis of *Aristolochia rathyae* collected from Arunachal Pradesh, north east India.

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Aristolochia (Family: Aristolochiaceae) is a highly valuable medicinal plant species distributed worldwide. About 500 species of *Aristolochia* are found globally, 20 have been reported from India with 7 species occurring in North-East India.[1] These species are ethnobotanically used to treat fever, stomach pain, dysentery, high blood pressure, malaria, headaches, coughs, and have other potential medicinal uses, including antifungal, antibacterial, and anti-inflammatory activities, along with nephrotoxic effects.[1] *Aristolochia rathyae* is an endemic species recently discovered from Kimin of Papum Pare district of Arunachal Pradesh, India.[2] The leaf samples of above plant were collected, dried and ground into fine powder. The petroleum ether extract of leaves was prepared, and used for GC-MS analysis. The GC-MS results identified more than 35 different compounds, such as Methacrylic acid ethyl ester, Acetic acid Butyl ester, Cyclotrisiloxane, Trans-3-Methyl-4-octanolide, D-Limonene, 2-(2-methoxyethoxy)propanoic acid, Nonanal, 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate, Neophytadiene, 2-Pentadecanone, 3,7,11,15-Tetramethyl-2-hexadecen-1-ol, Phthalic acid butyl undecyl ester, Tridecanoic acid, 4,8,12-trimethyl methyl ester, 1,2-Benzenedicarboxylic acid bis(2-methylpropyl), 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene, n-Hexadecanoic acid, Docosanoic acid ethyl ester, beta-D-Mannofuranoside, Palmitoleic acid, Phytol, Octadecanoic acid, 2-Propenoic acid, 3-methyl-5-(2,6-dimethylheptyl)-1,5-Pent-2-eno, Hexacosane, Bis(2-ethylhexyl) phthalate, Squalene, Heneicosane, Octacosanal, dl-α-Tocopherol, Nonacosan-14-one, 4,22-Stigmastadiene-3-one, and Cholest-4-en-3-one. The highest area percentage was recorded for Nonacosan-14-one (41.41%) at a retention time of 24.408 min. followed by 2-(2-methoxyethoxy) propanoic acid (8.97%), DL- α -Tocopherol (4.94%), Cholest-4-en-3-one (4.60%) and Butyl acetate (4.21%). These compounds possess potential medicinal and industrial applications in cosmetics and pharmaceutical products, skin-protection, as solvent in paint, varnishes and coatings, as antioxidant, food preservative, ink formulations, and fragrance carrier etc.

Key Words: *Aristolochia rathyae*, Arunachal Pradesh, GC-MS, Industrially valuable compounds.

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P-297

Investigation of Anticancer activity of self-assembled biocompatible glycoconjugates derived from Bhilawanol

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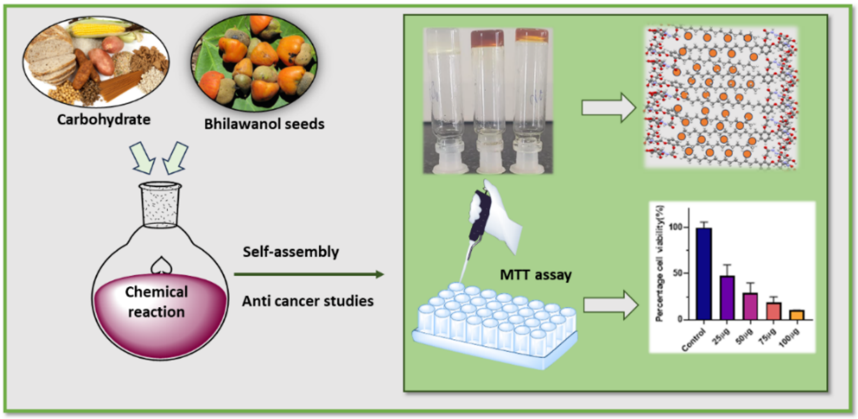
Cancer refers to a group of diseases marked by uncontrolled cell growth, leading to the formation of tumours, weakening the immune system, and potentially resulting in death. According to the World Health Organization (WHO), cancer is the second leading cause of death globally. This work focuses on developing an anti-cancer agent from natural molecules through supramolecular assembly. Our current approach centres on synthesising a new class of glycolipids from a renewable resource, bhilawanol (also known as urushiol), a bioactive molecule derived from *Semecarpus anacardium.* Bhilawanol-conjugated glycolipids (BCG) were synthesized by chemically modifying bhilawanol and linking it with monosaccharides, using a straightforward and eco-friendly process, and are well characterized by using different spectral techniques such as NMR, HRMS, IR, XRD etc. Developing carbohydrate-based glycolipids using simple synthetic methods is essential due to their biological and pharmaceutical relevance. The synthesised glycolipids were used to conduct an extensive anticancer study against HeLa cells.



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P-298

A new rhodamine isoindoline based fluorescent chemosensor for the detection of Fe (III) ions

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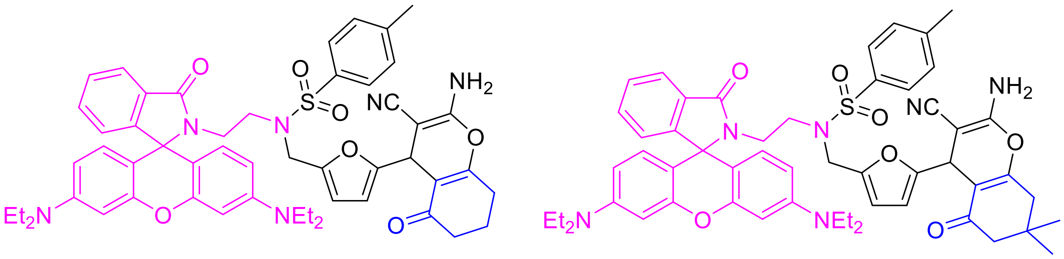
The design and synthesis of selective and sensitive chemosensors for the detection of metal ions have gained tremendous importance nowadays. [1] Rhodamine dyes have several applications in live cell imaging [2], single molecule imaging [3], and it can also be used as a thermometer for surface modification of viruses. In recent years, these dyes have been widely used as chemosensors in the detection of Hg^{2+}, Cu^{2+}, Fe^{3+}, Cr^{3+}, thiols, etc. [4]

Fe^{3+} is one of the most important ions which is especially involved in the formation of hemoglobin in the human body and various biological processes. It acts as a cofactor in many enzymatic reactions. [5] The deficiency of Fe^{3+} can affect the functioning of the heart, pancreas, and liver [6]. Overdose of Fe^{3+} may also induce a Fenton reaction, which produces reactive oxygen species, causing damage to nucleic acids, lipids, and proteins. [5]



Two novel rhodamine B-based fluorescent chemosensors containing isoindoline benzenesulfonamide moiety were designed and synthesized for the detection of Fe^{3+} ions. The UV-Vis and fluorescence spectral study showed that both of them can detect Fe^{3+} ions without interfering with other metal ions. They exhibited a 1:1 binding stoichiometry with the ion which was confirmed by Job's plot analysis. One of them is found to be more sensitive towards the Fe^{3+} ion with a detection limit of 59 nM. The fluorescence response to the addition of Fe^{3+} ion was attributed to the spirolactum ring opening of the probe. The binding mechanism was confirmed by DFT studies. The probe was also applied in the quantitative detection of Fe^{3+} ions in real water samples.

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P-299

Supramolecular Assemblies in Dicarboxylate based Metal-Organic Co-crystal Hydrates of Mn(II), Cu(II) and Ni(II): Combined Experimental and Theoretical Studies

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Metal–organic co-crystal hydrates; defined as the crystalline metal containing compounds with minimum two components along with uncoordinated water molecules; are so important in crystal engineering due to their potential applications in pharmaceutical and in synthetic organic chemistry [1]. It is also well established that dicarboxylic acids are often employed in crystal engineering of coordination compounds as they are excellent building blocks to construct network architectures through proton transfer and coordination to metal centers. The presence of two or more carboxylate moieties with different orientations allows the construction of interesting one-, two- or three-dimensional supramolecular network assemblies. In this context, coordination compounds of 2,6-Pyridine dicarboxylate, fumarate and isophthalate have been reported to possess numerous potential biological applications *viz.* anticancer, antibacterial and DNA binding properties [2]. Moreover, metal–organic compounds of pyridine-based ligands have been reported to display interesting biological applications [3]. 1,10-phenanthroline, is also capable of intercalating with DNA base pairs via aromatic □-stacking interactions due to the presence of rigid and planar polypyridine N-donor aromatic rings [4].

The weak forces of non-covalent interactions have prominent roles in the stabilization of bio-molecules like proteins, DNA and RNA. Among the well established non-covalent interactions, hydrogen bonding is one of the most frequently used interactions to develop supramolecular assemblies of desired dimensionalities. Non-covalent interactions involving the aromatic rings, *viz.* π-stacking, anion-π and C–H···π etc. can remarkably affect the properties of solid state self assemblies [5]. Again, H-bonded water aggregates and their enclathration within supramolecular hosts can direct the self-assembly process of coordination complexes and also facilitate the binding of the compounds with bio-molecules via supramolecular contacts [6].

Herein, we have reported the synthesis, crystal structures and characterization of three metal-organic co-crystal hydrates of Mn(II), Cu(II) and Ni(II), *viz.* $[Mn_3(2,6\text{-PDC})_4(H_2O)_4][Mn(H_2O)_6]\cdot 8H_2O$ (**1**), $[Cu_2(\text{□-fum})(\text{phen})_2(H_2O)_6](\text{fum})\cdot 6H_2O$ (**2**) and $[Ni(H_2O)_5(\text{DMAP})](\text{IPhth})\cdot 2H_2O$ (**3**) (where 2,6-PDC = 2,6-pyridinedicarboxylate, fum = fumarate, phen = 1,10-phenanthroline, DMAP = 4-dimethylaminopyridine, IPhth = Isophthalate). Crystal structure analysis of **1** and **2** unfolds the enclathration of $Mn(II)(H_2O)_6$ guests within the supramolecular host cavities and unusual infinite fum–water assemblies respectively. However, crystal structure analysis of compound **3** reveals the presence of various non-covalent interactions such as anion–π, π–π, C–H···π etc. which stabilize the layered assembly of the compound. The energetic attributes of the unusual supramolecular assemblies were theoretically examined, employing MEP surface analysis and the computational tools of combined QTAIM/NCI plotting. *In vitro* anticancer activities of compounds **1** and **2** considering cell viability and apoptosis assays against Dalton's lymphoma (DL) cancer cell lines reveal that the compounds induce considerable cytotoxicity in DL cells with negligible cytotoxicity in normal PBMC cells. Molecular docking was also conducted to investigate the potential interactions of the compounds with anti-apoptotic BCL family proteins.

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P-300

Highly conductive small *in situ* generated ligand-based metal organic frameworks

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Four isostructural formate based electrically conductive metal organic frameworks namely, $[H_2N(CH_3)_2][M(HCO_2)_3]$ (M=Mn; **Mn-F**, M=Co; **Co-F**, M=Ni; **Ni-F**, M=Zn; **Zn-F**), were synthesized with simple and cost effective methods. The *in situ* generated formate ion was attributed to decomposition of DMF, which was used as solvent of the reactions, under high pressure and temperature. Single crystal X-ray diffraction analysis reveals that MOFs also contain *in-situ* generated dimethyl ammonium cation inside their pores to maintain the charge neutrality of the framework. As-synthesized MOFs exhibit impressive room temperature electrical conductivity considering the electrical conductivity of MOFs reported so far. All the MOFs are semiconducting in nature and their conductivities increases with temperature. Again, Upon removal of guest from the pores the room temperature electrical conductivity of all the frameworks were improved except for **Co-F**. The theoretical evaluation of band of the MOFs reveals that through bond conductivity is siganificantly determined by the number of high spin electron in the metal d-orbitals.

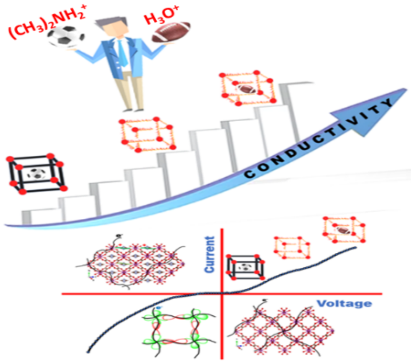

Figure. Graphical representation of the work.

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P-301

Synthesis of Copper MOF with carboxylic acid based ditopic linker for Efficient removal of organic dye from aqueous solution.

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Environmental contaminants from industries and human activities lead to a serious problem that requires our attention and we should find an efficient method to remove them from the environment[1]. Among many pollutants of water, organic dye is one of the major components which requires suitable attention as they are not only toxic but also non-biodegradable in nature and lead to serious environmental problems like carcinogenicity, mutagenicity, disability, reproductive defects etc. To remove these dyes efficiently from polluted water, we have synthesised a copper-based MOF which can effectively adsorb these organic dyes. This MOF was characterized by PXRD, FE-SEM, TEM, XPS, DSC and TGA. The surface area was determined by BET analysis. This MOF was used for the removal of organic dyes Methylene blue, Methyl orange and Rhodamine-B. These results will be presented in the form of a poster.

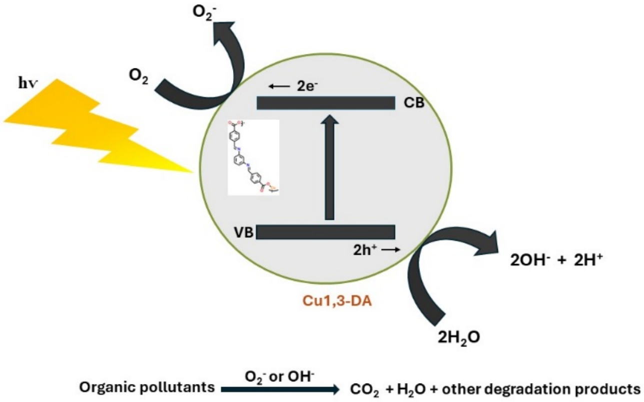

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Figure: - Photocatalytic degradation of Dye by Cu MOF.

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P-302

Molecular Docking and Dynamics of a Novel Inhibitor Targeting Mutant IDH1 in Cancer

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The mutant isocitrate dehydrogenase 1 (IDH1) enzyme has been identified as a target in cancer treatments, especially for cancers with abnormal metabolic activities like gliomas and AML[1]. Mutations in the IDH1 gene, particularly at amino acid R132, are linked to the production of 2-hydroxyglutarate, an oncometabolite that disrupts cellular differentiation[2][3]. A novel inhibitor has been designed to target this mutant IDH1 enzyme and analyzed through in silico methods. This study highlights the structural analysis and binding efficiency of the inhibitor. Molecular docking and dynamics simulations were conducted to assess the binding affinity and stability of the inhibitor, showing favorable interactions with key residues. The simulations confirmed the stability of the enzyme-inhibitor complex. Besides this, the ADMET predictions showed favorable pharmacokinetic properties, indicating the drug-like characteristics of the compound. These provide valuable insights into how inhibitors interact with mutant IDH1.

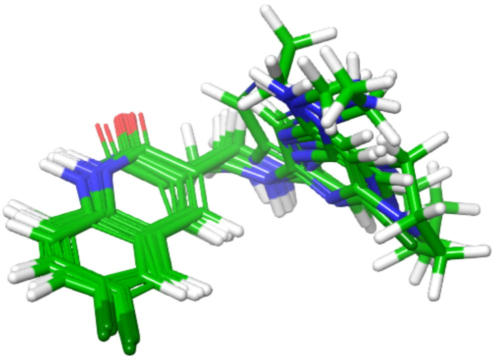

Figure: Molecular stacking image of designed molecules

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P-303

On the Accuracy of ML-BOP Model in Reproducing the Properties of High-Pressure Ices

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Water is one of the most complex substances in nature due to its anomalous behavior and has more than 19 different ice polymorphs, each having its unique properties. Simulating water's behavior, especially during phase transitions like crystallization and polymorphic transformation are computationally expensive when using all-atom models. That's where coarse-grained (CG) models come in—they are much more efficient, allowing us to simulate water at a fraction of the computational cost without sacrificing too much accuracy. One of the leading CG models is ML-BOP, a machine-learned bond-order potential based on the Tersoff potential [1]. This model has proven to be highly accurate in reproducing key thermodynamic properties of both liquid water and ice, such as temperature, enthalpy, entropy, and volume changes during melting. Not only is ML-BOP about 100 times faster than traditional models like TIP4P/2005 and TIP4P/Ice, but it also captures the structural changes between compact and open configurations under different temperature and pressure conditions, something critical for understanding water's complex behavior [2]. In this study, we assess the accuracy of the ML-BOP model for the thermodynamic and structural properties of high-pressure ices. We found that ML-BOP is able to reproduce the density and structure of the most common high-pressure ice phases. However, the lattice energy relative to ice Ih for most phases is overestimated by ML-BOP. Interestingly, ML-BOP predicts that ice Ih has the lowest lattice energy, in agreement with experimental results, which only a few empirical models can reproduce. Furthermore, we investigated the crystallization of ML-BOP water at very high pressures, in the region of high-pressure ices. Our results indicate that the explicit presence of hydrogen may be required to observe the crystallization of high-pressure ice and to correctly reproduce the stability of these ices. Overall, ML-BOP performs better than another popular coarse-grained mW model [3-4] of water in reproducing high-pressure ice properties.

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P-304

Iron-Catalyzed Synthesis of Ferrocenyl-thioether Conjugates via C-S Cross Coupling of Thioethers and Vinyl Chlorides: Construction, Anticancer and Computational Studies

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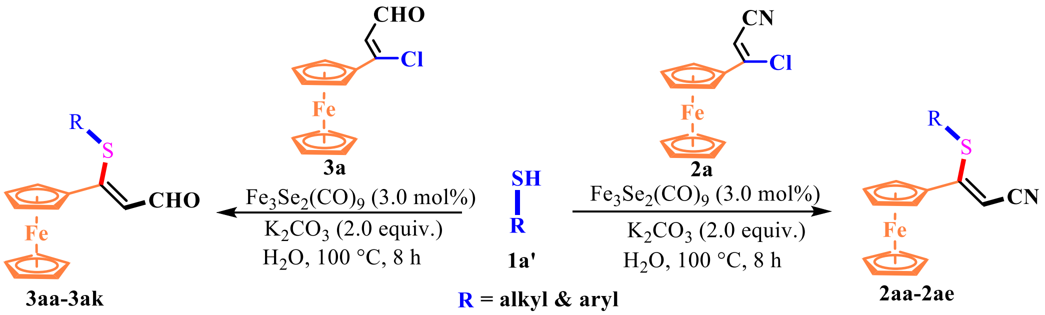
Herein, a library of ferrocenyl-thioether derivatives of acrylaldehyde and acrylonitrile has been developed via a direct C-S bond formation reaction under mild conditions. Various aromatic and aliphatic thiols were successfully coupled with ferrocenyl acrylaldehyde/acrylonitrile [1,2] in presence of a catalytic amount of chalcogen-stabilized iron carbonyl cluster ($Fe_3Se_2(CO)_9$). All the reactions were carried out in water under aerobic-conditions and transformed a wide range of ferrocenyl-thioether derivatives in good yield. Furthermore, the cytotoxic studies of some selected ferrocenyl-thioethers were investigated against the Prostate cancer cell lines (PC-3) and normal human embryonic kidney cell lines (HEK). 3-Ferrocenyl-3-(4-trifluoromethyl)-phenylsulfanyl was found to be significantly active, it showed IC_{50} 5.5 µM towards prostate cancer cell lines [3], moreover, it also showed a comparable activity with standard anticancer drugs including axitinib, nelfinavir, and thymitaq, and (±) thioridazine. Anticancer activity was further supported by DFT calculations including the HOMO─LUMO energy gap, cyclic voltammetry (CV), UV-Vis studies, molecular docking and reactive oxygen species (ROS) analysis. All the compounds reported in this report are new and they may serve as milestone in the futuristic research of anticancer drug.



Scheme 1. Iron catalyzed S-vinyl-thiolation of ferrocenyl *β*-chloro acrylaldehyde/acrylonitrile with thiols

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P-305

ε-Poly-L-lysine: A Naturally Occurring Biodegradable Polypeptide for Selective Detection of 5-Nitroimidazole Antibiotics in Animal Products and Living Cells via Fluorescence

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The 5-nitroimidazole (5-NI) class of antibiotics, such as metronidazole, ornidazole, secnidazole, and tinidazole, are widely used to prevent bacterial infection in humans and livestock industries. However, their overuse contaminates the farmed animal products and water bodies. Hence, a selective, sensitive, and cost-effective method to detect 5-NI antibiotics is the need of the hour. Herein, we report a rapid, inexpensive, and efficient sensing system to detect 5-NI drugs using an as-prepared solution of ε-poly-L-lysine (ε-PL), a naturally-occurring and biodegradable homo-polypeptide that has an intrinsic fluorescence *via* clustering-triggered emission (CTE). The low nanomolar detection limit (3.25-3.97 nM) for the aforementioned representative 5-NI drugs highlights the sensitivity of the system outperforming most of the reported sensors alike. The resulting fluorescence quenching was found to be static in nature. Importantly, excellent recovery (100.26%-104.41%) was obtained for all real samples and animal products tested. Visual detection was demonstrated using paper strips and silica gel for practical applications. Furthermore, ε-PL could detect 5-NI antibiotics in living 3T3-L1 mouse fibroblast cells through cellular imaging. Taken together, the present work demonstrates the detection of 5-NI antibiotics using a biocompatible natural polypeptide, ε-PL and represents a simple and inexpensive analytical tool for practical application.

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P-306

A hydrazine-free photoredox catalytic synthesis of azines by reductive activation of readily available oxime esters

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Herein, we present a novel, hydrazine-free photoredox catalyzed platform for azine synthesis using mild, simple reaction conditions. While previous energy transfer activations of oxime esters lead to decarboxylation of the O-auxiliary and radical combination with the iminyl radical, the reductive electron transfer strategy herein affords high yields of azines using only a triarylamine organophotocatalyst and no additives. Scale up was readily achieved by means of a continuous flow reactor. Mechanistic studies indicate a preassembly of photocatalyst and substrate is key to achieving efficient and selective N–N iminyl radical coupling.

P-307

Regioselective Synthesis of 4-Arylamino-1,2-Naphthoquinones in Eutectogel as a Confined Reaction Media using LED Light

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Abstract

Predicting the selectivity and conversion in a confined reaction media under photochemical condition is highly challenging as compared to the conventional synthesis. Supramolecular assembly is a ubiquitous phenomenon in nature in which molecules spontaneously form aggregates *via* non-covalent interactions, which intrinsically able to control selectivity, rate of conversion and kinetics of a chemical process in biological systems.[1] We have synthesized hydroxymethyl derivative of Dibenzylidene sorbitol (DBS) gelator, which can self-assemble itself in deep eutectic solvents (DES) and there by forming eutecto-gels. DES are composed of a Lewis or Brønsted acids and bases displaying intermolecular H-bonding, which facilitate substantial depression in freezing point. Nevertheless, a direct phase change of DES system into liquid ensures its application in organic synthesis & catalysis. Our conceptual approach utilizes the use of one of the interesting natural compounds, Lawsone (2-hydroxy-1,4-naphthoquinone) as one of the starting materials, which display a broad range of biological and pharmacological properties. we report the use of a DBS derived eutectogel facilitating a LED light induced regioselective synthesis of 4-arylamino-1,2-naphthoquinones in good yield. This protocol realizes the challenging photochemical reaction in a confined gel media using simple and mild conditions. Herein, we introduce a comprehensive method based on the regioselective photochemical reaction in eutectogel Predicting the selectivity and conversion in a confined reaction media under photochemical condition is highly challenging as compared to the conventional synthesis.

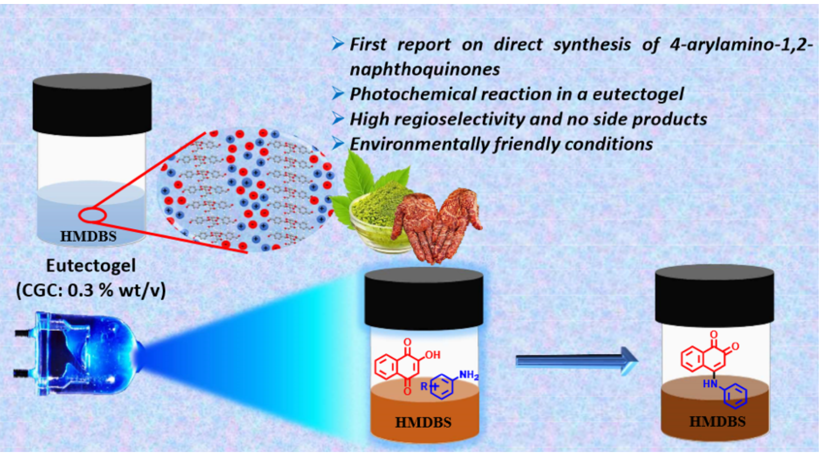

Figure 1. The use of a simple eutectogel derived from carbohydrate facilitating a LED light induced regioselective synthesis of 4-arylamino-1,2-naphthoquinones in good yield is reported

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P-308

Folic Acid and Cyclodextrin Functionalized Silk fibroin-capped Gold Nanoparticles for Targeted Delivery of Anticancer Drug

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Cancer is one of the leading causes of mortality worldwide and is treated through various approaches, including radiation therapy, chemotherapy, and surgical intervention(1). Among these, chemotherapy remains a widely utilized treatment modality through the administration of anticancer drugs. However, conventional chemotherapy is associated with several limitations, such as poor target specificity, limited drug bioavailability, solubility issues, drug resistance, and systemic toxicity(2). Consequently, the development of targeted drug delivery systems (TDDS) has become increasingly important in overcoming these challenges and enhancing therapeutic outcomes. In this study, we have developed a TDDS with SF (silk fibroin) in its backbone. The SF backbone was functionalized with CD (β-cyclodextrin) for enhanced bioavailability and solubility and Folic acid (FA) for target specificity. Further, the modified SF was capped over gold nanoparticle (AuNP) to produce CD-SF-FA@Au nanoparticle. The nanoparticle was further characterized to find the structure and stability. The synthesized CD-SF-FA@Au NP was loaded with model drug and had a loading efficiency of 93.5%, significantly higher than conventional cyclodextrin-based drug carriers. Further, its in-vitro release study was performed.

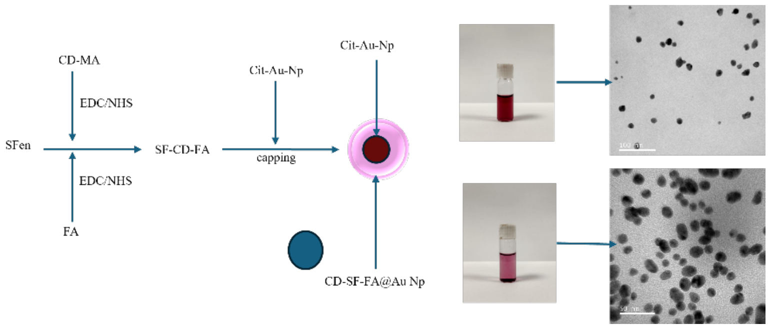

Figure 1. Graphical abstract for the synthesis of SF-CD-FA capped gold nanoparticle.

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P-309

Organocatalytic Asymmetric Synthesis of Carbo- and Oxa-Cyclic Seven-Membered Bridged-Biaryls *via* Domino Sequence

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Despite the ubiquitous occurrence of biaryl-bridged seven-membered scaffolds in valuable natural products, bioactive compounds, chiral catalysts and molecular motors, their asymmetric synthesis remained underdeveloped.[1] The seven-membered bridged-biaryl framework possesses more configurational stability than the related smaller ring structures and could be resolved as atropisomers. Acquainted with the importance of developing asymmetric methods for acquiring a biaryl-bridged seven-membered skeleton, we have proposed a switchable reactivity for the asymmetric synthesis of dibenzocycloheptanes and 5,7-dihydrodibenzo[*c,e*]oxepines. Thus, a new class of substrate bearing two different acceptor sites at the two *ortho*-positions of the biaryl rings has been developed to undergo organocatalytic asymmetric 1,4-/1,2-addition or 1,2-/1,4-addition reactions depending on the nucleophile type to access seven-membered carbo- or oxa-cyclic biaryl bridged compounds bearing multiple chiral centres and a chiral axis in a highly stereoselective manner.[2] In continuation of our interest in developing medium-sized bridged biaryls, we have utilized bifunctional H-bonding organocatalysts to procure oxindole-bearing seven-membered carbocyclic bridged biaryl with multiple stereocenters and a chiral axis. In this case, two acceptor sites undergo domino 1,2-/1,2 addition from the same carbon of the nucleophile to provide an efficient entry to seven-membered carbocyclic products with excellent enantio-and diastereoselectivity.[3] The findings of our research in these endeavours will be presented in detail.

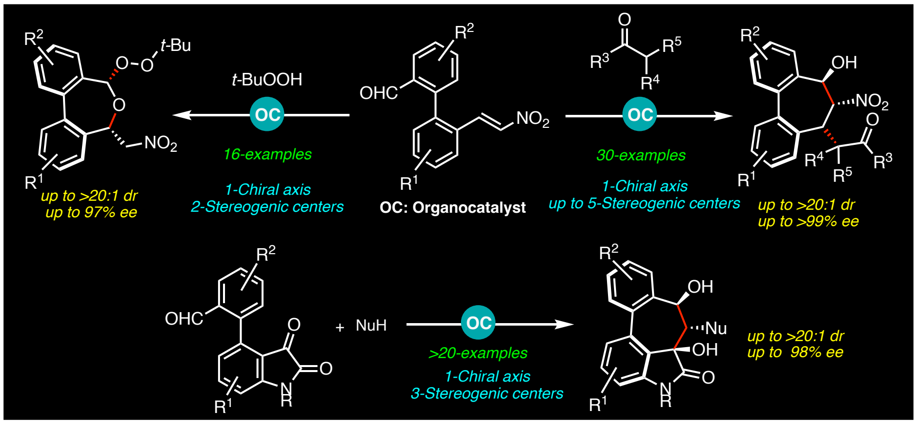

Figure 1. Asymmetric Synthesis of Biaryl Bridged Seven-membered Carbo- and Oxa-cyclic Frameworks.

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