Recent Advances on Materials for Sustainable Energy

International Symposium

Theme: Small Molecule Activation

Book of Abstracts

RAMSE
2025

13 December 2025

Organized by: Department of Chemistry and Chemical Biology
IIT(ISM) Dhanbad, Jharkhand, INDIA-826004

Recent Advances on Materials for Sustainable Energy

RAMSE 2025

Theme: Small Molecule Activation

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One Day symposium Organized by:

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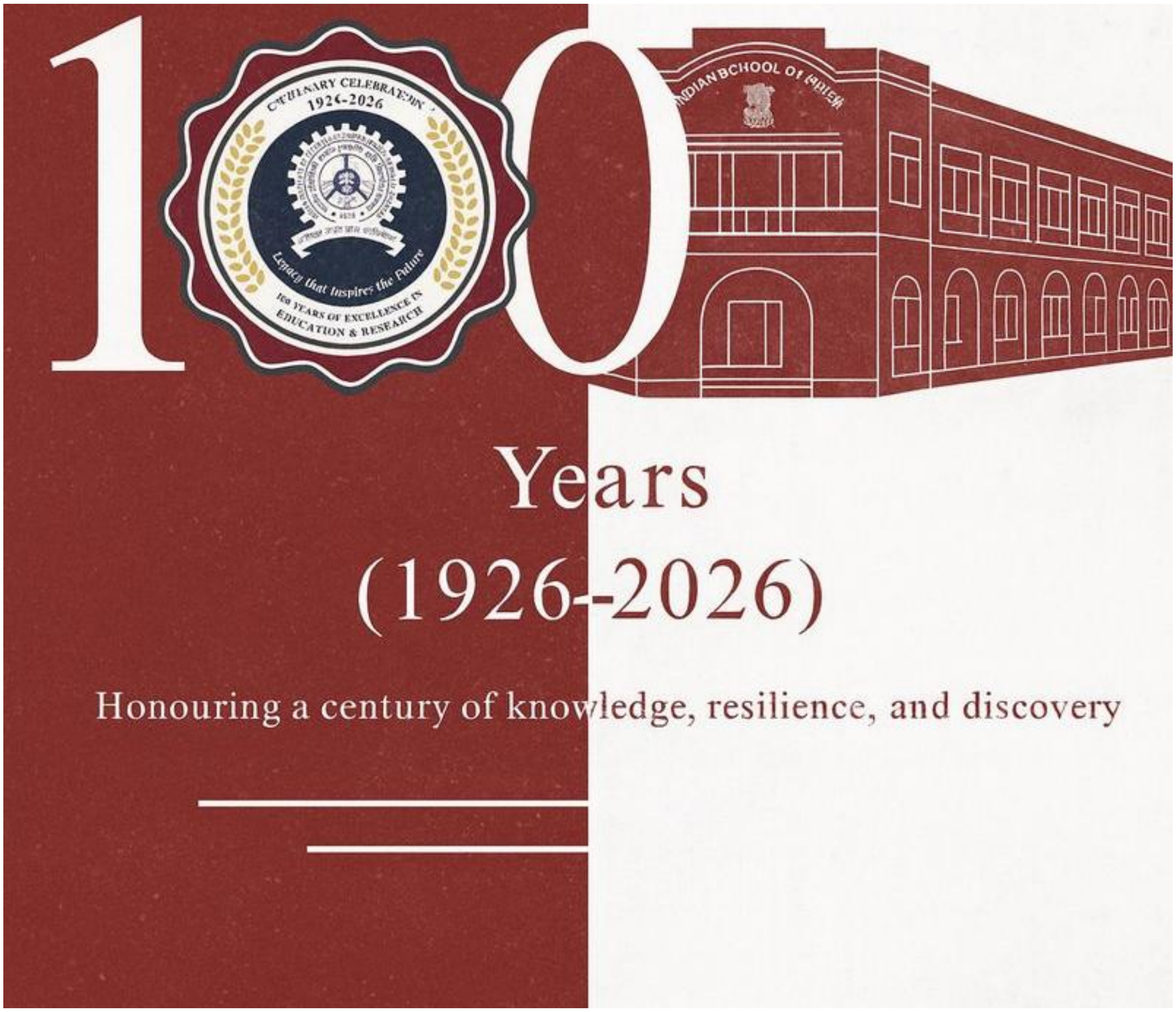

Programme

Time	Session	Speaker
7:30 AM – 8:30 AM	**Breakfast at EDC Dining Hall**	
9:00 AM – 9:30 AM	Inauguration Ceremony (Welcome Address & Opening Remarks)	
Session I	**Chair: Prof. D. D. Pathak**	
9:30 AM – 10:30 AM	Invited Talk I	Prof. Ebbe Nordlander
10:30 AM – 11:30 AM	Invited Talk II	Prof. Bhabani S. Mallik
11:30 AM – 12:00 PM	Invited Talk III	Prof. Pankaj K. Koli
12:00 PM – 12:30 PM	Invited Talk IV	Prof. Prasenjit Mondal
12:30 PM – 1:00 PM	Invited Talk V	Prof. R. Mayil Murugan
1:00 PM – 3:00 PM	**Lunch Break & Poster Session** **(At the I2H building basement.)**	
Session II	**Chair: Prof. R. P. John**	
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4:00 PM – 5:00 PM	Invited Talk VII	Prof. Sukanta Mandal
5:00 PM – 5:30 PM	Invited Talk VIII	Prof. Subhendu Naskar
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INVITED TALKS

RAMSE-2025

Department of Chemistry and Chemical Biology
IIT(ISM) Dhanbad

Influence of stereoelectronic effects on hydrogen atom and oxygen atom transfer reactions involving high-valent iron-oxo complexes

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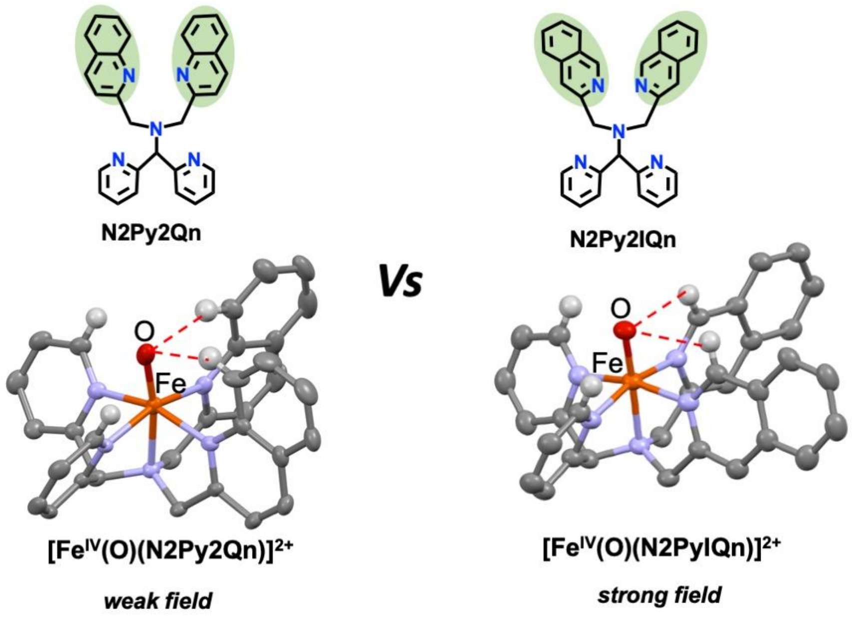
The roles of high-valent iron-oxo intermediates in a number of heme[1] and non-heme[2] oxygenases are well-established. Several Fe(IV)=O complexes have been synthesized as biomimetic models for such intermediates.[3] This lecture will discuss the steric and electronic effects of various equatorial substituents on the hydrogen atom and oxygen atom transfer reactivities of $[Fe(IV)=O(L^5)]^{2+}$ complexes, where L is a pentadentate N5-donor ligand based on the N4Py framework, and of $[Fe(V)(O)(OH)(L^4)$ complexes, where L is a tetradentate N4-donor ligand.



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Mechanistic and Biomimetic Studies of Nitrate and Nitrite Reduction to Nitric Oxide

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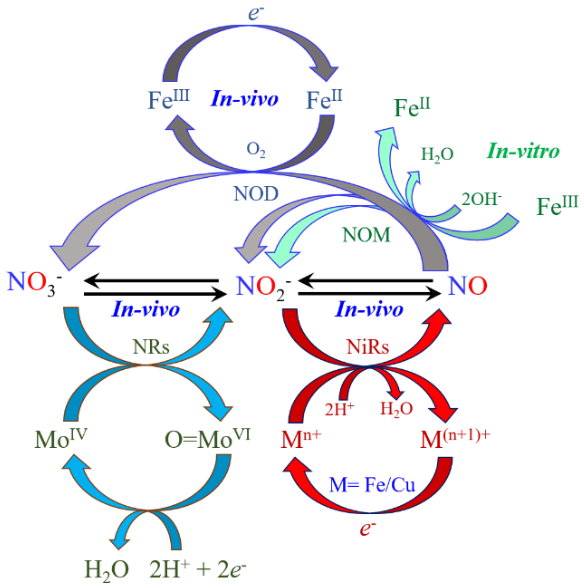
Nitric oxide (NO) plays a crucial role in various physiological processes, including neurotransmission, vascular regulation, platelet aggregation, and immune response to multiple infections.[1] Therefore, to maintain an optimal concentration of NO, nitrate reductase (NR), nitrite reductase (NiR)[2], and NO synthase (NOS)[3] enzymes are available for NO biosynthesis. If overproduced, NO Dioxygenase (NOD) enzymes convert NO to biologically benign NO_3^-. The reductive process of NO biosynthesis begins with NR, which catalytically transforms NO_3^- to NO_2^- via the O-atom transfer (OAT) reaction using Mo/W-based enzymes. Meanwhile, NiR enzymes catalyze the conversion of NO_2^- to NO in the presence of acid (H^+).[2] Here, we will explain the reduction of NO_2^- to NO via acid-induced reaction on Co/Fe/Cu centers.[4] A new pathway for NiR enzyme activity was observed with one equivalent proton (H^+) generating M-NOs (or NO generation) with H_2O_2 (which further decomposes to H_2O). Also, VCl_3-induced NO_3^-/NO_2^- reduction was confirmed on the Co-center.[5] In addition, we will also be presenting the NO oxidation reaction of $\{CoNO\}^8$ to understand the mechanistic aspects of base-induced NO mono-oxidation to NO_2^- with H_2 evolution.[6]



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Electrochemical Activation of Small Molecules by Tuned Water Dynamics

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The transition to a sustainable and decentralized chemical economy critically depends on efficient electrocatalytic small molecule activation (SMA). The electrode potential leads to a strong interfacial electrical field, which significantly increases the water-reorganization energy, and thus affects the electrochemical activation of small molecules at the interface through the proton/hydroxide transfer in the electrical double layer (EDL). Other factors, such as electrostatic interactions and water dynamics, also have been proposed to contribute to the catalysis.[1] In addition, the solvation of reaction species can also crucially contribute to the reaction free energy at electrified interfaces. The interfacial hydrogen-bond networks may play a critical role in the kinetics of interfacial proton-coupled electron transfer reactions. Traditional computational methods often treat the electrode potential implicitly, which is insufficient for accurately modeling complex electrochemical reactions. Neglecting water dynamics near interface[2,3] will not provide accurate dynamic facilitated catalytic reaction mechanism. However, by employing constant potential molecular dynamics, the presentation will elucidate the atomistic mechanisms, potential-dependent reaction free energy landscapes, and identify crucial electrocatalytic descriptors like water dynamics and double-layer structure.[4] The insights gained are vital for the rational design of more efficient, selective, and durable electrocatalysts, accelerating the development of sustainable energy and chemical production technologies.

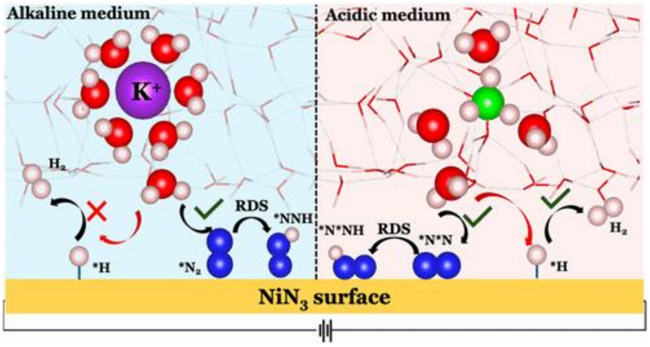

Figure 1: The representative structure of the NiN3/H2O electrode-electrolyte interface in (a) acidic medium represented with H_3O+ (green colour) and (b) alkaline medium represented with KOH

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Copper(II) catalyzed oxidative amination and etherification reactions: Mechanistic rationalization using computational approach

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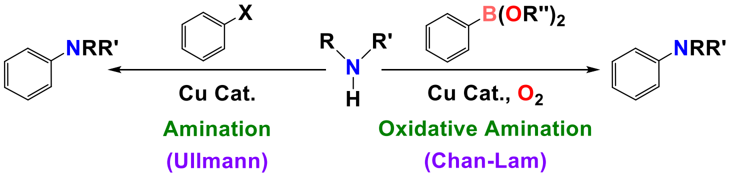
Methodology for carbon-nitrogen (C–N) bond formation is an active field of research for organic synthesis because nitrogen containing compounds are necessary building scaffolds for useful pharmacophores and bioactive compounds.[1] Transition metal-catalyzed C–N cross-couplings are broadly based under two sections: the classical nucleophile-electrophile coupling characterized by the Ullmann-Goldberg reaction and the oxidative nucleophile-nucleophile coupling, the Chan-Evans-Lam (CEL) amination as represented in Scheme 1.[2,3] The current presentation will discuss a detailed mechanistic investigation, employing the state-of-the-art quantum mechanical calculations, of the C–N and C–O bond formation reactions within the Cu^{II} catalyzed CEL protocol.[4] The calculations will broadly provide an overview of the following fundamental steps in the catalytic transformation: catalyst activation, transmetalation, disproportionation, reductive elimination and finally oxidation to generate the monomeric Cu^{II} catalyst.[4] Furthermore, the role of transmetalated byproduct $B(OH)_3$ in circumventing the use of additional base will also be discussed. The modified protocol shows enhanced efficiencies towards amination and etherification reactions in presence of less effective aryl boronic acid pinacol esters.[3]



Scheme 1. Copper catalyzed C–N cross-coupling reaction.

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Water Oxidation Catalysis by Rationally Designed Ruthenium Complexes

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The production of hydrogen by splitting water utilizing sunlight presents a promising solution to the world's increasing energy demands and environmental challenges. Water oxidation is considered the most challenging among the various steps involved in water splitting. Developing highly efficient water oxidation catalysts (WOCs) has become pivotal in renewable energy research. Ruthenium-based complexes have emerged as promising catalysts due to their unique combination of enriched redox properties, robust nature, and superior catalytic performance compared to other transition metal-based molecular catalysts. The presentation will showcase the chemistry of water oxidation reactions catalysed by newly developed ruthenium complexes.[1-4] It will explore the critical role of ligand design, emphasising the benefit of incorporating redox-non-innocent character within the supporting ligands and fine-tuning the secondary coordination sphere.

$$2H_2O \xrightarrow{\text{Ru-WOCs}} O_2 + 4H^+ + 4e^-$$

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Transition Metal Complex based Electrocatalysts for OER, HER and CO2RR Activity

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Search of sustainability in energy encourages researcher to explore multiple aspects of energy production and storage. Development of catalyst is one key factor while considering a renewable energy production through electrochemical or photochemical means. Both homogeneous and heterogeneous method of catalysis are important as the former provides mechanistic information, while the later is better for practical application. Production of hydrogen through water splitting comprises of two complementary processes: water oxidation and proton reduction.

Transition metal complexes are well known catalysts for these purpose. 1st row transition metals e.g., Co, Ni and Cu with redox non innocent Pyridyl, imidazole and amide ligands have been utilized to get the novel catalysts which have been explored in homogeneous and heterogeneous catalysis. A series of Cu complexes of bis-amide tetradentate ligands show efficient electrocatalytic water oxidation with a TOF of 1462 s^{-1} at overpotential~700 mV. Stepwise ligand-centered oxidation process and the. Stepwise ligand centered oxidation process and the formation of the O─O bond during water oxidation passes through the water nucleophilic attack for all the copper complexes. Another water soluble binuclear aquo Cu(II) amide complex shows ternary role as an electrocatalyst for the OER, HER and CO2RR. Electrokinetic parameters for HER was calculated as follows: TOF = 1679 s^{-1}, TON = 586 and F.E. = 83%. With a F.E. of 92%, CO2RR shows percentage selectivity of ~99.99% conversion of CO2 to $(COOH)_2$.M terpyridine complexes have been explored for their efficient electrocatalytic activity in homogeneous medium which maintains their integrity at the extreme pH levels. A series of terpyridine complexes have been explored for the OER and HER study in solution that displays high degree of stability as confirmed by different surface characterization techniques e.g. FESEM, TEM etc. (for electrodes) and DLS (for solution). An attempt to immobilize a Cu terpyridyl complex on the GC electrode surface leads huge increment in the current density compared to the homogeneous medium. When the catalyst is mixed with Graphene oxide and immobilized on Glassy carbon electrode, ~70 times increase in current intensity at the catalytic wave is noticed at an overpotential of ~407 mV.

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Bioinspired Aromatic Hydroxylation: Role of Redox-Active Metals

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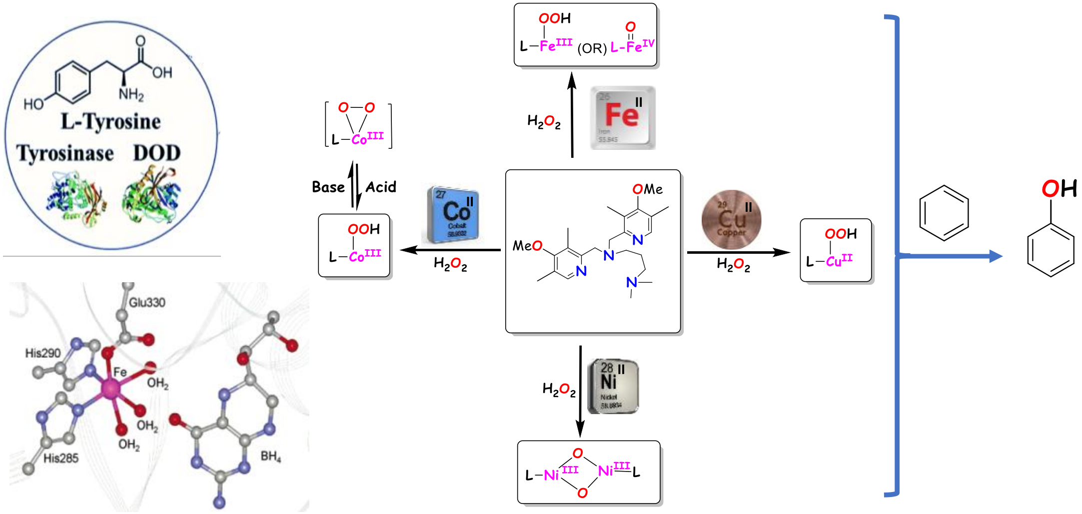
Phenol is the starting material for synthesizing several industrially valuable chemical products. It is manufactured only by a three-step cumene process using benzene and dioxygen, which shows a yield of ~ 5%. Therefore, developing a single-step methodology is crucial for synthesizing phenol from benzene. Its high C-H bond energy (460 kJ mol−1) and the lack of kinetic control of phenol oxidation over benzene hamper the higher yields. However, naturally occurring oxygenases are known to activate these C-H bonds at ambient conditions using dioxygen. We have reported the Ni(II) complexes of N_4 ligands $[Ni^{II}(N_4)(CH_3CN)_2]^{2+}$ as bioinspired catalysts for benzene hydroxylation. It showed a maximum of 41% phenol formation using H_2O_2 as an oxidant by the involvement of short-lived key intermediate species $[(N_4Ni^{III})_2(\mu\text{-}O)_2]^{2+}$. However, the Co(II) complexes of the identical ligands favored Co(III)-hydroperoxo for the benzene to phenol conversion, which showed only a 29% yield. Interestingly, the Cu(II) complexes of the same ligand series afforded 37% of phenol from benzene via Cu(II)-OOH intermediate. The Fe(II) analogs showed a 21% yield of phenol occurred via $[(L)Fe^{III}\text{-}OOH]$ species or its high-valent species. The ligand architecture and redox potentials varied the catalytic efficiency of complexes. Our methodology is the new biomimetic catalytic process for phenol formation from benzene via the greener pathway at a single step.



Scheme 1. The metalloenzymes are known to perform hydroxylation (left) and benzene hydroxylation reactions by our bioinspired catalysts (right).

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Terminal Ligands in Controlling the Stability and Reactivity of Mononuclear Cu(III) Complexes

***Chinmay Parida*[a]*, Alok Panigrahi*[a]*, Amirul Islam*[a]*, <u>Prasenjit Mondal</u>**[a]*

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Great efforts have been made to generate new types of late transition metal oxidants by tuning terminal ligands.[1-5] These metal oxidants play a key role to activate and functionalize C–H bond *via* proton coupled electron transfer (PCET) reactions.[1-5] Herein, we have developed unique oxidants, high valent metal-cyanate/azide, at room temperature. The high valent mononuclear complexes $[(L)Cu^{III}(X)]$ ($X = OCN^-$, $N3^-$; H_2L = N,N′-(2,6-diisopropylphenyl)-2,6-pyridinedicarboxamide) were prepared from $[(L)Cu^{II}(X)]Bu_4N$ by one electron oxidation under ambient conditions (**Figure 1**) and both complexes were characterized by X-ray crystallography and UV-vis, $^1H/^{13}C$ NMR, Raman, FT-IR and EPR spectroscopies, ESI-MS. At room temperature, high valent complexes reacted with C–H bond in hydrocarbons and phenolic O–H bond via hydrogen atom transfer mechanism, as evidenced by kinetic data and product analysis. The reaction rates of these complexes with substrates are comparable to some reported reactive metal oxidants. Fascinatingly, complexes performed direct C–N bond formation by activating C–H bond and radical capture reactions. Our results found new class of metal oxidants for strong C–H bond functionalization.

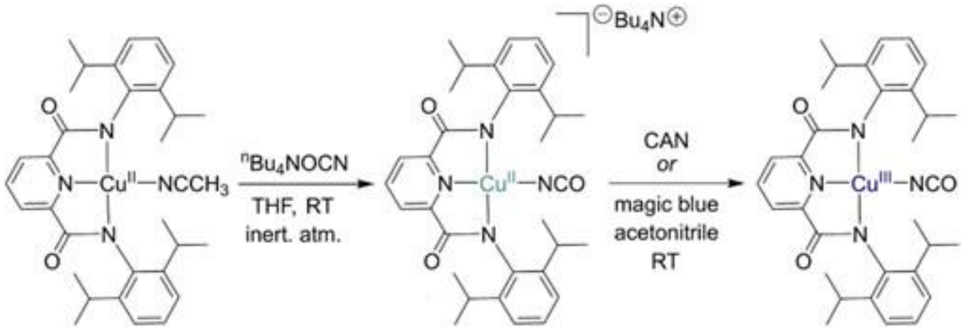

Figure 1. Preparation of high valent Cu-complexes.

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NITRIC OXIDE-INDUCED LIGAND DISPLACEMENT IN COBALT PORPHYRIN SYSTEMS

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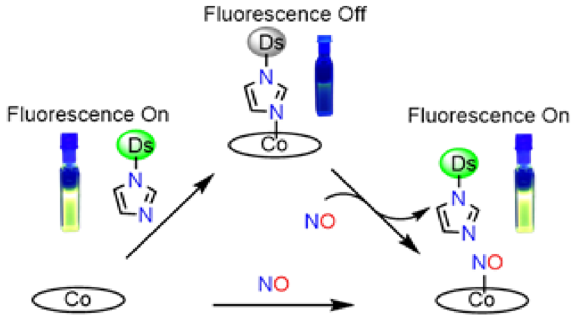
Nitric oxide (NO), the tiny biological signaling molecule, is a molecule of wonders as it is simultaneously vital to life and potentially harmful too, depending on its concentration. A slight variation in the concentration, the bio-friendly NO suddenly becomes lethal.[1-4] The short half-life, low physiological levels, and highly reactive nature of NO imply a significant challenge for its selective detection. Hence, developing a highly selective molecular probe for NO will indeed help with its qualitative and quantitative estimation. Here, we report a Co^{II}-based fluorescent probe [(Imi-Ds)Co^{II}-TMPP] (2) (TMPP = tetra-methoxyphenyl-porphyrin) prepared by functionalizing [Co^{II}-TMPP] (1) with imidazole-dansyl (Imi-Ds) fluorophore ligand, which detects NO by employing a fluorophore displacement strategy. Imi-Ds fluorophore ligand showed >95 % fluorescence quenching (turn-off) upon binding to complex 1 compared to the free ligand ($\Phi = 59\%$). Complex 2 showed the formation of [(NO)Co-TMPP] (3), $\{CoNO\}^8$) in the presence of NO via the displacement of Imi-Ds fluorophore, thereby restoring fluorescence emission by ≈ 90 % (fluorescence turn-on). Fluorescence studies using reactive nitrogen and oxygen species (RNS/ROS) indicate that complex 2 exhibits high selectivity for NO *via* a fluorophore-displacement mechanism, enabling both qualitative and quantitative detection. The Probe shows a detection limit of ≈ 10 nM, which suggests its better and enhanced sensitivity performance for NO sensing applications.



Scheme 1: Nitric oxide-induced fluorophore displacement

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GO-APTMS-Cu(II) schiff base immobilized graphite rod for hydrogen evolution reaction in water

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Abstract- Hydrogen evolution reaction (HER) using 3d metal based electrocatalysts is one of the field being highly explored. Herein we synthesized two GO (graphene oxide) based electrocatalysts, **1** and **2** immobilized on graphite rod for the reduction of protons to dihydrogen in aqueous medium. This strategy developed low cost electrodes for HER. The schiff base catalysts are synthesized using *4-(diethylamino)-2-hydroxybenzaldehyde* and *3,5-di-tert-butyl-2-hydroxybenzaldehyde* with (3-Aminopropyl)trimethoxysilane (APTMS) on the GO matrix. Using perchloric acid in aqueous media with the modified graphite rods generates H_2 with high efficiency and stability. The 21.5 hours of chronopotentiometry of the electrodes exhibited mild fluctuation in the voltage for **1>2** deduces that **2>1** in terms of stability. The CV plots exhibited a current denisty of 0.0045 A/cm^2 for **2** and 0.003 A/cm^2 for **1** showcase **2** in HER activity while exhibiting a TOF of 8.4 s^{-1} and 124 s^{-1} respectively. The TON observed for **1** and **2** are 3×10^4 and 4.4×10^5 with F.E of 37.6% and 52.5% respectively. DLS was used to observe the stability of the electrodes. TGA identified the higher thermal stability of **2** than **1**. Gas chromatography analysis after CPE at -1.3 V vs Ag/AgCl and -1.7 V vs Ag/AgCl for **1** and **2** respectively is found to be in agreement with the electrochemical paradigm.

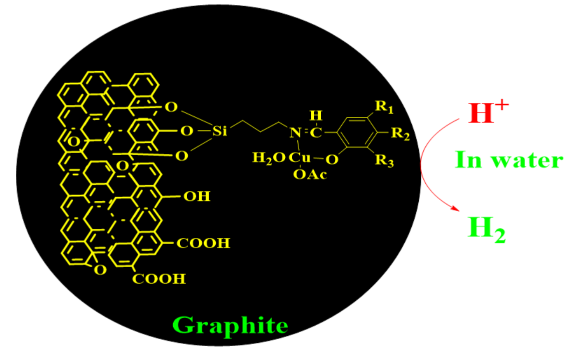

Figure 1- Schematic diagram of reduction of protons to Hydrogen through modified graphite electrodes.

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Mechanistic Divergence in Sulfur-Ligated Iron(III)-Alkylperoxo Reactivity: Aldehyde Oxidation Prevails over Deformylation

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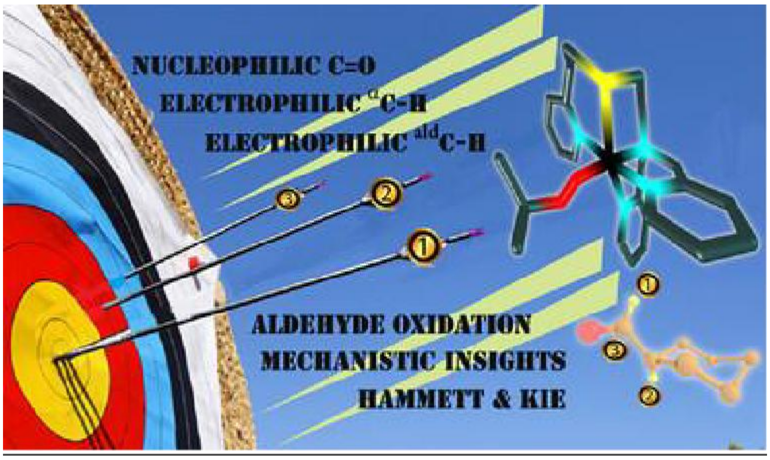
Metalloenzymes activate molecular oxygen within their catalytic cycles to generate a reactive species capable of substrate transformation. In many iron-containing enzymes, it is a high-valent iron(IV)-oxo complex that is synthesized from an iron(III)-alkylperoxo intermediate, although direct observation and characterization of such species have remained elusive, leaving their mechanistic role uncertain. To address this gap in our understanding, we present here the synthesis, comprehensive characterization, and reactivity of a novel thioether-ligated iron(III)-alkylperoxo complex supported by the ligand 2-((2-(pyridin-2-yl)ethyl)thio)-N,N-bis(pyridin-2-ylmethyl)ethan-1-amine. Characterization was done using UV–vis spectroscopy, resonance Raman spectroscopy, electron paramagnetic resonance spectroscopy, and electrospray ionization mass spectrometry. Reactivity studies reveal that this complex exhibits electrophilic oxidation of model substrates, including dimethylsulfide, triphenylphosphine, and cyclohexanecarboxaldehyde. Notably, the latter substrate reacts via the unusual aldehyde C─H bond abstraction leading to cyclohexanecarboxylic acid, which is explained by favorable aldehyde C─H abstraction transition states due to stabilizing interactions between the ligand framework and the substrate. Moreover, the reaction is initiated with a homolytic O─O bond cleavage in the iron(III)- alkylperoxo group that yields a reactive iron(IV)-oxo species that mediates substrate oxidation. To our knowledge, this work represents the first example of a mononuclear low-spin (S = ½) nonheme iron(III)- alkylperoxo complex displaying such unprecedented electrophilic reactivity.



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Water-Soluble Arene-Ru(II) Half-Sandwich Complexes For Efficient Ammonia Borane Dehydrogenation Via Hydride Intermediate

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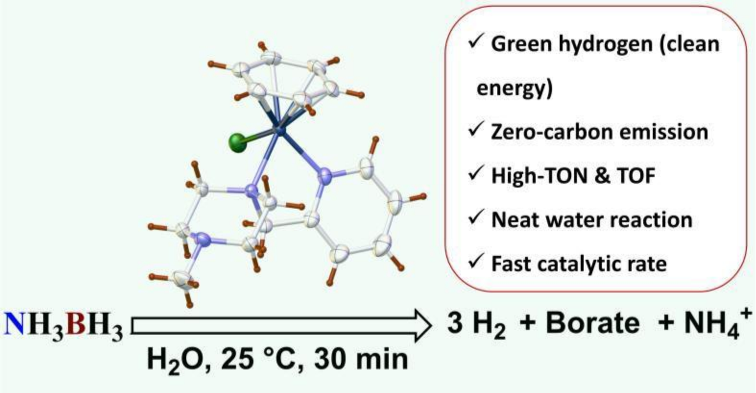
A series of water-soluble arene-Ru(II) complexes (**Ru1-Ru3**) was synthesized and fully characterized by spectroscopic techniques, and their molecular structures were confirmed by single- crystal X-ray diffraction. These complexes efficiently catalyze the dehydrogenation of ammonia borane (AB) at 25 °C, completing H_2 release within 30 min, as quantified by online GC analysis. Kinetic studies using differential pressure manometry revealed first-order dependence on both [Ru] and [AB]. A key hydride-Ru(II) intermediate was identified by ^1H NMR and mass spectrometry, supporting the proposed mechanism. The catalysts exhibit excellent durability, remaining active over nine consecutive cycles without significant loss of performance. Among them, (**Ru2)** showed the highest activity, delivering the fastest rates with a turnover number of 247, a turnover frequency of 494 h^{-1}, and up to 2.95 equiv. of H_2 released from ammonia borane ($NH_3.BH_3$).



Scheme 1. Ruthenium(II)-catalysed dehydrogenation of ammonia borane at room temperature.

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Electrochemical CO$_2$ reduction to formic acid using molecular Cobalt (II) complex

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The electrochemical reduction of carbon dioxide (CO$_2$) to value-added chemicals presents a promising pathway for sustainable carbon management. Here, we report a homogeneous cobalt-based molecular electrocatalyst [Co(N3Q3)(H_2O)Cl]Cl {where N3Q3 =N,N-bis(quinolin-8-ylmethyl)quinolin-8-amine} that selectively converts CO$_2$ to formic acid with high efficiency by utilizing 3.3 M of H_2O as a proton source. The catalyst exhibits a remarkable Faradaic efficiency of 88% toward formic acid formation, demonstrating strong product selectivity and minimal competitive hydrogen evolution. Kinetic analysis reveals an impressive turnover frequency TOF$_{max}$ of 1440 s^{-1}, highlighting the rapid catalytic turnover enabled by the cobalt center and its tailored ligand environment. Our studies confirm that ligand N3Q3 is highly effective in converting CO$_2$ to HCOOH via 2H$^+$/2e$^-$ reduction process with an overpotential of 330 mV *vs.* SCE. Structural and electrochemical investigations suggest that the catalyst through a Co(II)/Co(I) pathway that facilitates CO$_2$ insertion and proton-coupled electron transfer. This work underscores the potential of molecular cobalt systems as efficient, tunable, and scalable platforms for homogeneous CO$_2$ reduction, advancing the development of next-generation electrocatalysts for carbon- neutral fuel and chemical production.

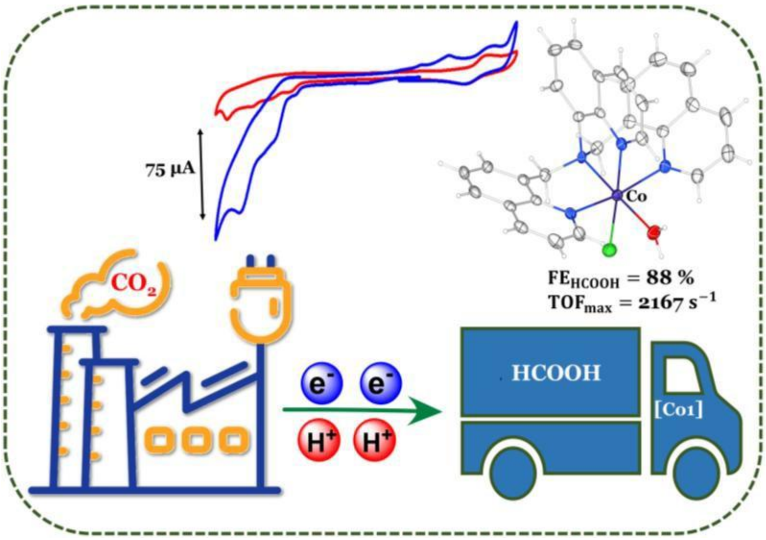

Figure 1: Cobalt based molecular catalyst for electrochemical CO$_2$ reduction.

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Cascade C─ H-Alkenylation-Intramolecular Aminative Cyclization of Benzylsulfonamides for Synthesis of Isoindoline Cores

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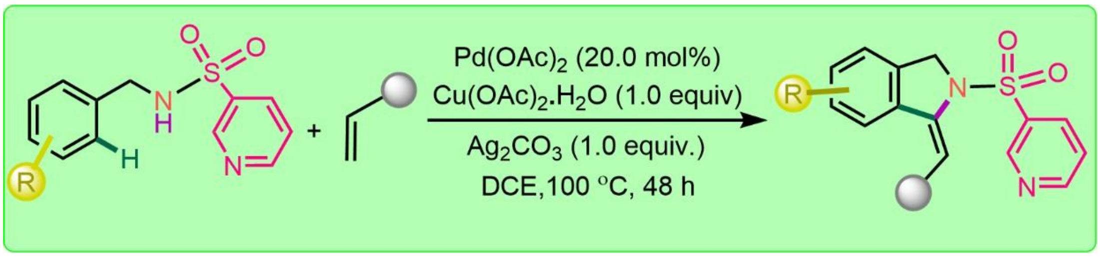
Isoindoline-core-bearing compounds are pharmaceutically relevant compounds against a myriad of diseases. Traditionally, the isoindoline core is synthesized from benzylamines by two-step synthesis involving *ortho*-C-H alkenylation followed by acid or metal-catalyzed cyclization. Herein, we execute a direct synthesis of the isoindoline core by a one-step procedure involving the *ortho*-C-H alkenylation- oxidative amination mediated cyclization of pyridine-sulfonamide derivatives of benzylamines with acrylates and sulfones via Pd-Ag bimetallic catalysis.



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Terpyridine-Mediated Organo-Electrocatalytic CO_2-to-CO Reduction Explored by DFT

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New and sustainable energy vectors are required as a consequence of the environmental issues associated with the continued use of fossil fuels, with electro-catalytic CO_2 reduction becoming a key focus. We report here a series of CO_2 reducing electrocatalyst based on substituted terpyridine derivatives(**L1-L6**) that are very selective for production of carbon monoxide in dimethylformamide (DMF)/H_2O mixtures. Faradaic efficiency of (74 ± 10%) at moderate overpotentials (650−850) mV vs. SCE. Conversion of CO_2 into value added product using polypyridyl ligand is very rare. Notably, catalyst **L6** demonstrated impressive faradaic efficiency (FE) for CO and H_2, with 74% and 0.04% at -1.8 V vs. SCE, respectively, after 3 hours of electrolysis. All these catalysts, **L1-L6**, exhibit over 90% selectivity for CO generation. The DFT studies reveal that the mechanism follows EECC pathways, where 'E' represents electrochemical steps and 'C' denotes chemical steps.

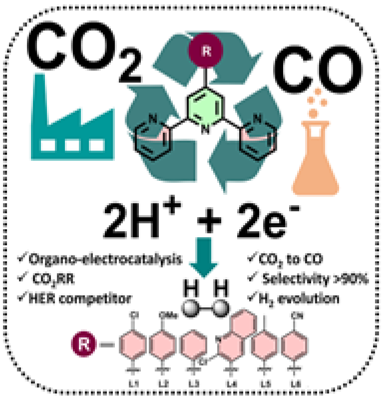

Figure 1: Selective CO_2 Reduction Using Homogeneous Organo-catalysts.

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Hypervalent Group 14 compounds as catalysts for Organic Transformation

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Hypervalent compounds of the heavier Group 14 elements, particularly tin and germanium, have emerged as versatile catalysts for a wide range of organic transformations. Their unique electronic structures—characterised by expanded valence shells and three-centre–four-electron (3c–4e) bonding—endow these species with pronounced Lewis acidity and tuneable coordination geometries. Over the past few years, our group, with innovative ligand design and controlled hypervalent frameworks, have enabled Sn(IV) and Ge(IV) compounds to mediate reactions such as C–C and C–N bond formation, hydrosilylation, Diels-Alder cycloaddition, and hydroboration. The ability of these systems to stabilise high-coordinate environments while maintaining reactive apical sites makes them promising alternatives to traditional transition metal catalysts. Current research continues to expand the scope and mechanistic understanding of hypervalent main group elements, highlighting their potential in developing efficient, cost-effective, and environmentally benign synthetic methodologies.

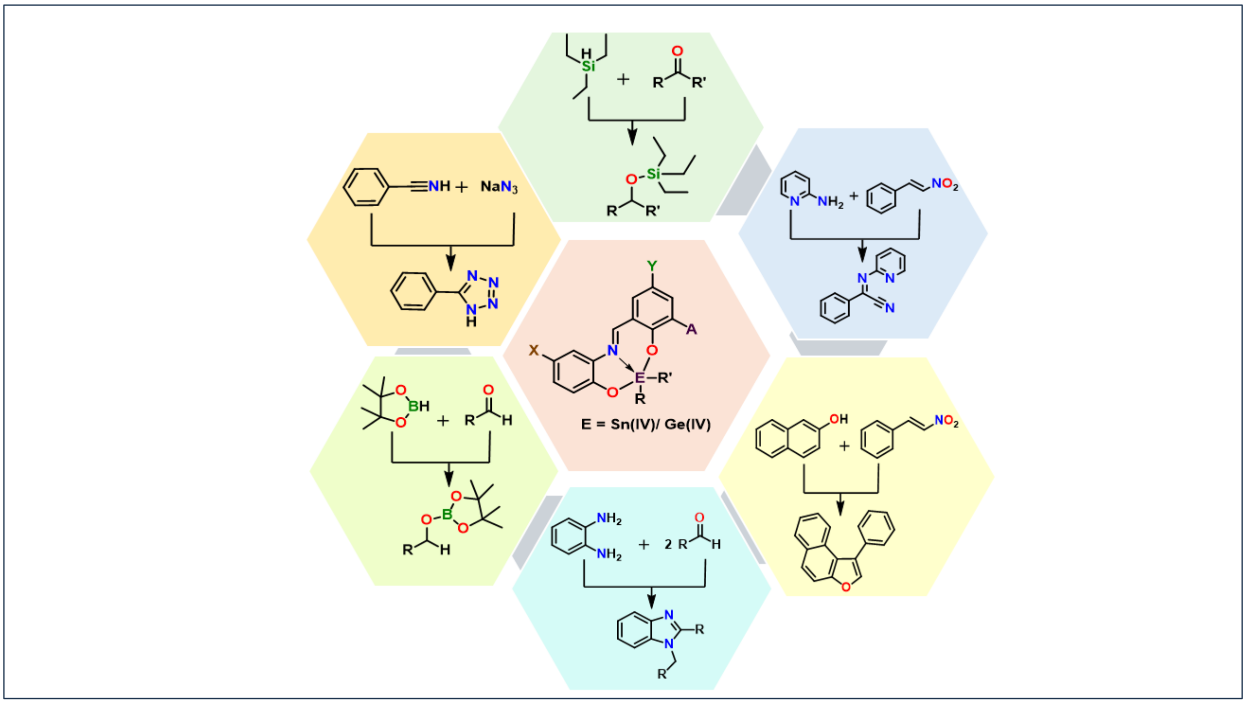

Fig. 1: Hypervalent Group 14 compounds as catalysts for various organic transformations.

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One pot synthesis of Fe doped $CoWO_4$ as a novel electrocatalyst for water oxidation in alkaline medium

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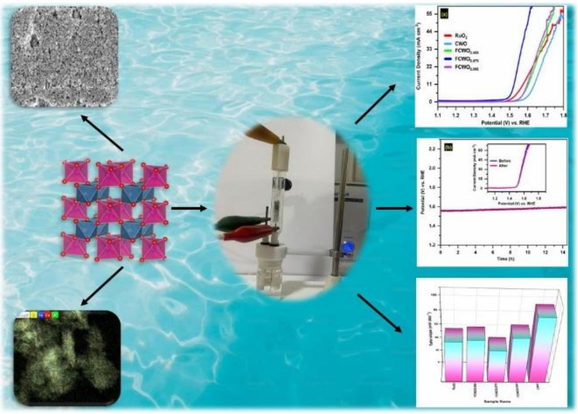
Electrochemical water splitting can be a game-changer in the field of non-conventional energy systems owing to its numerous benefits. In this study, a facile hydrothermal synthesis of $CoWO_4$ having semi-amorphous nature with doping of Fe in different concentrations is reported. Initially, the samples were thoroughly characterized, prior to being tested as a potential catalyst for oxidation of water in alkaline medium. Electrochemical evaluation proclaims that 75 mg doping of Fe in $CoWO_4$ represented as $FCWO_{0.075}$ exhibits maximum catalytic activity and a reasonable overpotential of 292 mV at a current density of 10 mA cm^{-2}. The synergistic effect between Co and Fe amplified the activity of $CoWO_4$ after doping with iron. A significant effect on specific surface area of it after doping is evident in BET isotherms, possibly contributing to the enhancement in activity of the as-prepared catalyst $FCWO_{0.075}$. The BJH plot reveals that it is mesoporous in nature having pore size of 10.62 nm. In addition to it, smaller Tafel slope as 49.46 mV dec^{-1} and higher mass activity measured at different overpotentials, ECSA values out performing ever RuO_2 proves its excellence as a catalyst. Moreover, it also possesses a substantial durability of ~15 h in chronopotentiometry (CP) and 2000 cycles of CV with no obvious decay in potential.



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Pd(II)-Catalyzed One-Pot Oxidative Heck/C–H Arylation Cascade Enabling Access to 3–Nitro–2–Arylindoles

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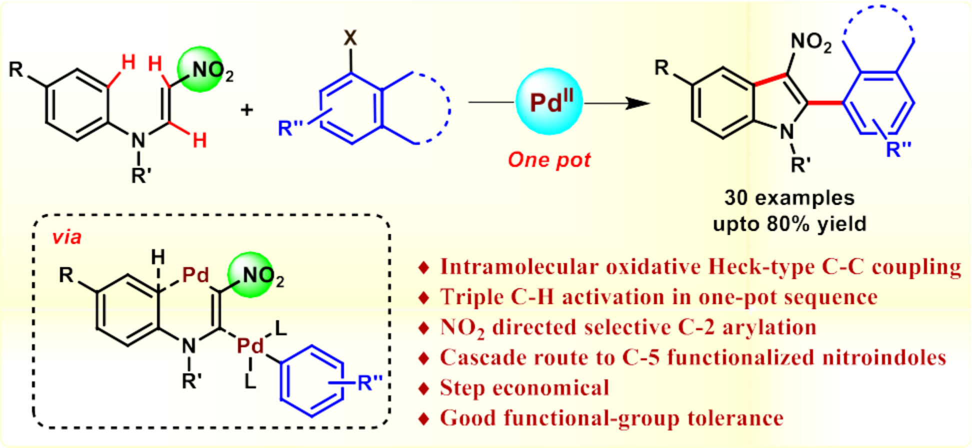
The present study discloses a Pd(II)-catalyzed one-pot cascade process that enables rapid access to **C-2-aryl-3-nitroindoles** from readily available *N*-aryl nitro enamines and haloarenes. The transformation proceeds *via* an intramolecular oxidative Heck-type C–C coupling to generate a 3-nitroindole intermediate in situ, followed by **NO_2-directed C-2 arylation**, all under a unified catalytic system. This atom-economical protocol delivers a broad array of **C-2-aryl-nitroindole scaffolds** in good to excellent yields and is readily applicable to the streamlined synthesis of **C-5-functionalized** derivatives bearing F, Cl, Me, and OMe substituents. Mechanistic studies—supported by radical trapping, control and competition experiments, and EDG/EWG analysis—indicate a pathway involving triple **C–H activation, σ-bond metathesis or base-accelerated proton abstraction**, leading to a key **Ar–Pd–C-2-nitroindole** intermediate. The results highlight the directing ability of the NO_2 group in governing reactivity and regioselectivity, establishing this cascade as an efficient platform for the preparation of nitroindole motifs of pharmaceutical interest.



Scheme 1: Pd(II)-driven dual C–C bond formation delivering 3-nitro-2-arylindoles.

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Integrated MnCo-MOF-5/rGO as Hierarchically Mesoporous Electrode for High-Performance Asymmetric Supercapacitor and Theoretical Validation of MnCo-MOF-5 Structure

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Herein, a one-pot solvothermal method was adopted to fabricate a marigold-like trimetallic MOF (Zn, Co, Mn; MCM) on reduced graphene oxide (rGO).[1,2] The MCM structure was validated by the DFT optimization with a band gap of 2.9698 eV, against the experimental value of 3.0298 eV. BET isotherm hysteresis indicates a 2.44 times enhancement of the specific surface area of MCM-rGO composite (MCM 200) compared to MCM. Three-electrode study of MCM demonstrates specific capacitance of 66.46 F g^{-1} at 2 A g^{-1} current density in 1M TEABF$_4$/DMSO electrolyte.[3] For the asymmetric supercapacitor of MCM 200, a specific capacitance of 181.5 F g^{-1} (290.4 C g^{-1}) was obtained at 0.2A g^{-1} with an energy density of 64.53 Wh/Kg. An unusual increase of specific retention up to 178% was observed after 12000 charge-discharge cycles. The power law and Trasatti method revealed that MCM 200 follows both double-layer-controlled and pseudocapacitance charge transfer mechanisms, respectively.[5] Moreover, three ASC devices were able to power the combined multi-colour LEDs after 60 seconds of charging at 4.8 V. After the cyclic stability test, the disassembled MCM and MCM-200 electrodes were post-characterized using PXRD, FE-SEM with point EDX, and XPS analyses. The results confirmed that the electrodes retained identical structural morphology to the as-synthesized materials.

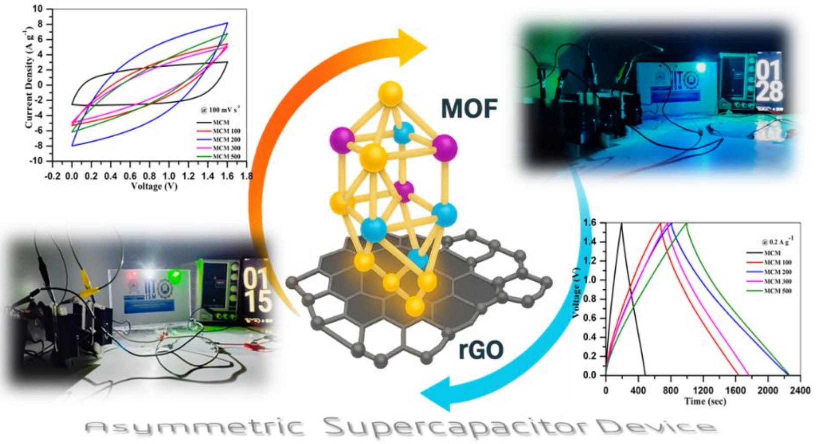

Figure: Diagrammatic representation of the MCM 200 electrode material for a high-energy Asymmetric supercapacitor.

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HER performance by CuMn-P/NF electrocatalyst in alkaline medium

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Generation of carbon neutral and clean fuel like hydrogen has become immediate necessity to eradicate both energy depletion and environmental problems. Surge in development of bimetallic phosphide catalysts on nickel foam as substrate has been observed in the recent times. Herein we report a bimetallic phosphide catalyst, CuMn-P/NF for its HER performance in alkaline aqueous medium of 1M KOH. Electrode preparation is a simple one-step electrodeposition of bimetallic phosphide system on nickel foam as substrate. Freshly prepared catalyst showed around 200-fold increase in activity with respect to nickel foam. At 10 mA cm^{-2} the catalyst showed an overpotential of 405 mV with an overall good stability in highly alkaline medium.

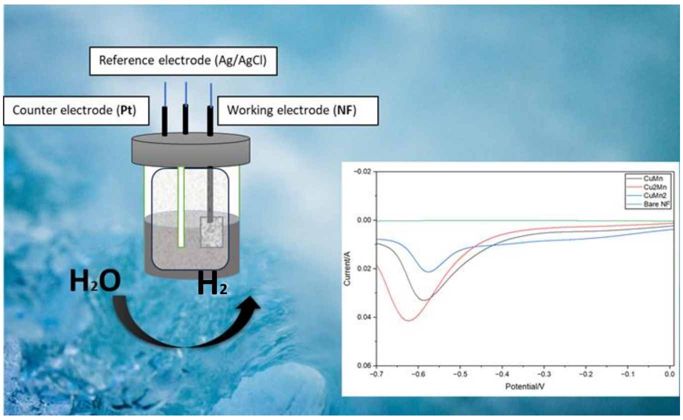

Figure 1: Schematic diagram of hydrogen evolution by CuMn-P/NF catalyst.

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Visible Light Assisted Photocatalytic Removal Of Bisphenol A By Bismuth Niobate/g-C_3N_4 Heterojunction

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Persistent organic pollutants (POPs), such as bisphenol A (BPA), provide significant risks to environmental and human health, even at negligible concentrations[1]. We engineered a high-performance visible-light-driven $BiNbO_4$/g-C_3N_4 heterojunction through the strategic thermal optimization of bismuth niobate synthesis using a solvothermal-calcination approach[2, 3]. Temperature-dependent phase engineering (300-900 °C) demonstrated significant structural transitions: Bi_3NbO_7 (300-500 °C) to $Bi_5Nb_3O_{15}$ (600-700 °C) to orthorhombic $BiNbO_4$ (≥°C), with peak solar photocatalytic activity attained at 500 °C (Eg = 2.36 eV). The creation of heterojunctions using g-C_3N_4 markedly diminished crystal lattice strain, improved charge carrier mobility, and facilitated dual Type II/Z-scheme electron transport pathways[4]. Composite $B_{1.5}G$ displayed superoxide radicals ($*O_2^-$) as the primary active species for BPA degradation in sunlight whereas $BG_{1.5}$ showed excellent response to LED light through a combination of $*O_2^-$ and hole oxidation pathways[5]. The obtained BPA degradation as function of reaction rate constant is presented in Figure 1 This study illustrates methodical material design for the activation of small-molecule pollutants and sustainable water treatment in accordance with SDG 6 objectives.

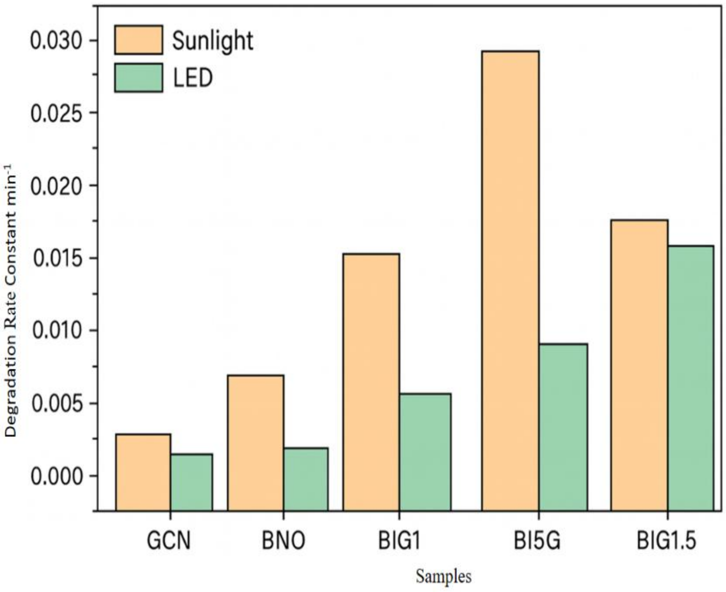

Figure1. BPA degradation presented as a function of degradation rate constant

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Ruthenium-Doped Mixed Sulphide Catalyst In-Situ Engineered for Efficient Urea Oxidation and Hydrogen Production

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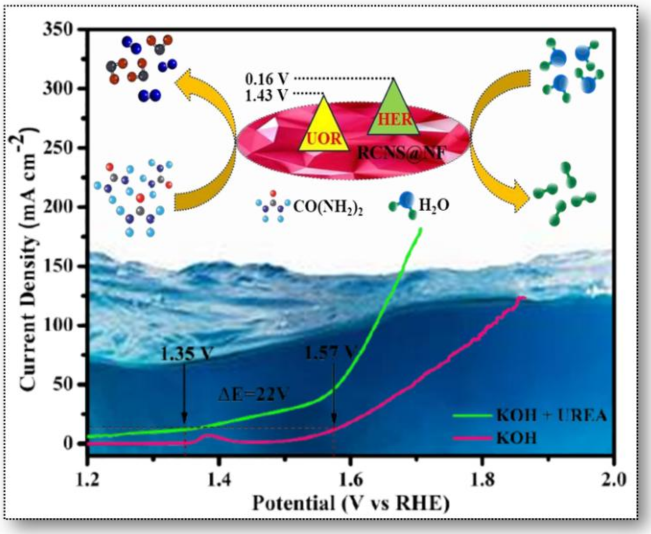
Growing global energy demands, depletion of fossil fuels, and increasing environmental concerns have intensified the need for clean and sustainable energy alternatives. Hydrogen, with its zero carbon emissions, high gravimetric energy density, and excellent energy conversion efficiency, is considered one of the most promising future fuels. Electrochemical water splitting offers a green and efficient route for producing high-purity hydrogen; however, its practical implementation is challenged by sluggish kinetics and high overpotentials associated with the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). To overcome these limitations, replacing OER with the thermodynamically favourable urea oxidation reaction (UOR, 0.37 V) presents a highly energy-efficient approach. In this work, we report an in-situ engineered Ru-doped bimetallic sulphide catalyst synthesized via a hydrothermal process followed by calcination. The catalyst features a pyramid-like nanostructure with enhanced crystallinity and strong synergistic effects, enabling excellent bifunctional activity. It achieves 20 mA cm^{-2} at just 1.43 V for UOR and requires an ultralow overpotential of only 16 mV (vs. RHE) to reach 10 mA cm^{-2} for HER. A symmetric two-electrode configuration delivers 10 mA cm^{-2} at a low cell voltage of 1.35 V and maintains stable performance for 20 hours. These results demonstrate the strong potential of this Ru-doped sulphide catalyst for energy-efficient hydrogen generation via urea-assisted electrolysis.

Graphical Abstract:



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Mononuclear Lanthanide(III) Complexes for Efficient Conversionof CO_2 to Cyclic Carbonates

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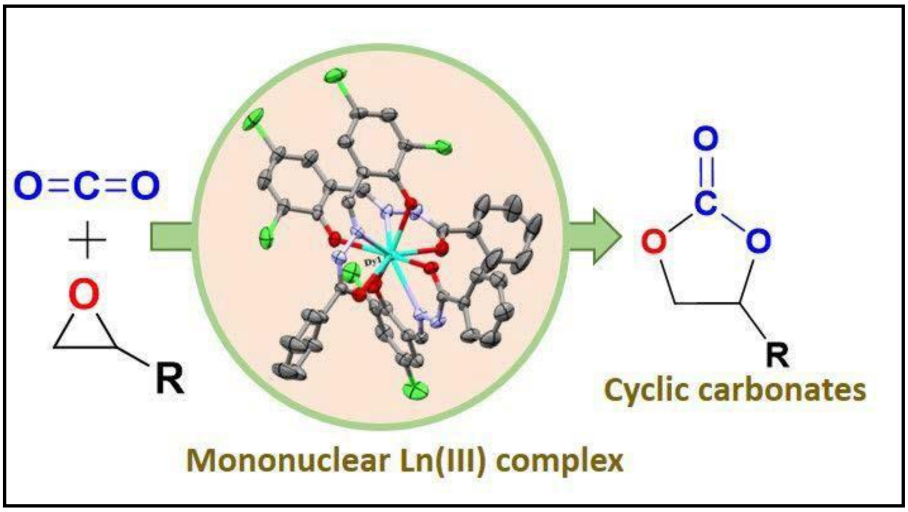
Two new mononuclear lanthanide(III) compounds, formulated as $[(HL)_3Dy]\cdot MeOH\cdot H_2O$ **(1)** and $[(HL)_3Er][Et_3NCl]\cdot H_2O$ **(2)**, were synthesised via the reaction of a polydentate pro-ligand H_2L with the corresponding hydrated lanthanide(III) chloride salts in the presence of triethylamine as a base under ambient methanolic conditions. The complexes were thoroughly characterised by elemental analysis, FT-IR spectroscopy, powder X-ray diffraction, and single-crystal X-ray diffraction, the latter confirming the mononuclear nature of both lanthanide centres. Compounds **1** and **2** exhibit significant catalytic activity in the cycloaddition of CO_2 to epoxides, affording cyclic carbonates in good yields under solvent-free conditions. The influence of substituents on the reactivity of various epoxides toward CO_2 fixation was also systematically examined. Based on these findings, a plausible catalytic mechanism for the cycloaddition reaction has been proposed. These results highlight the potential of structurally well- defined mononuclear lanthanide complexes as efficient catalysts for conversion of CO_2 to cyclic carbonates.



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Hybrid Co(II) Coordination Polymer/CNT/GO Electrodes for High Energy Asymmetric Supercapacitor

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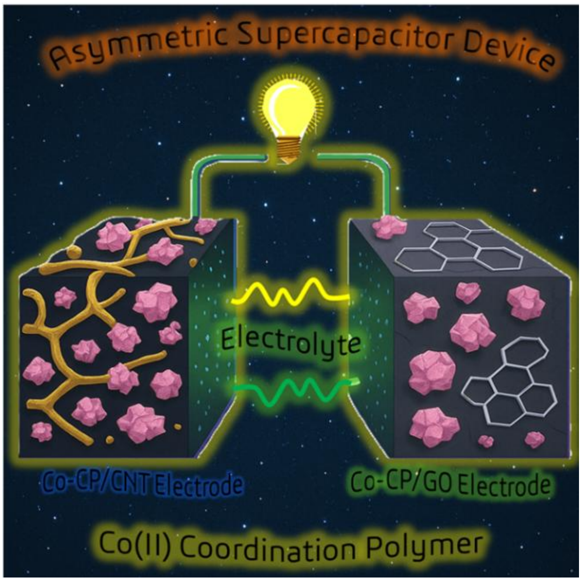
Two-dimensional (2D) coordination polymers (CPs) have garnered increasing interest in electrochemical energy storage due to their planar architectures, which facilitate enhanced interfacial interactions with 2D carbonaceous materials. Herein, we report the solvothermal synthesis of a Co(II)-based coordination polymer, $[Co(PDA)(H_2O)]_n$ (namely, MCo). The structure of MCo was elucidated by single-crystal X-ray diffraction (SC-XRD), revealing an ***hnb***-type underlying net topology. The morphology and chemical composition of the resulting composites were characterized by FESEM, HR-TEM, and XPS analysis. Electrochemical analysis of symmetric supercapacitors (SSC) and asymmetric supercapacitors (ASC) showed that the ASC device has a higher specific capacitance (Sp.CP). The specific capacitance of MCo, MCo/CNT 100, and MCo/GO 20 was calculated to be 14.54, 287.13, and 373.12 F g^{-1} at a current density of 0.5 A g^{-1}, respectively. The energy density and power density of MCo/GO 20 were found to be 132.6 Wh kg^{-1} and 400 W kg^{-1} at 0.5 A g^{-1}. The ASC device retained 68% of its capacitance after 10,000 charge-discharge cycles, demonstrating good cyclic stability. For a practical demonstration, the ASC device successfully powered red, multicolor disco, and white LEDs, maintaining illumination for 120 seconds after charging for 60 seconds. These results highlight the potential of the MCo/GO 20 composite as a promising electrode material for next-generation supercapacitor applications.



Graphical Abstract: Effect of 1D and 2D carbonaceous materials over 2D inorganic-organic coordination polymer for asymmetric supercapacitor device.

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Engineering a High-Performance Electrocatalyst for Efficient Oxygen Evolution Reaction

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The design of economical and efficient electrocatalysts is essential for advancing electrochemical water splitting and sustainable energy technologies[1,2]. In this study, a nanostructured transition-metal oxide catalyst ($NiMoO_4$) was synthesized through a hydrothermal method, yielding well-defined rod-like structures decorated with spherical nanoparticles. The dual incorporation of Fe and Co into the oxide lattice effectively tailored its electronic configuration, resulting in enhanced charge transport and improved electrical conductivity. The optimized catalyst achieves a current density of 10 mA/cm^2 at a low overpotential of 239 mV in alkaline electrolyte. The improvement in electrochemically active surface area stems from the synergistic interactions among the dopant metals and the lattice framework, along with the contributions of its hierarchical nanomorphology. Furthermore, the catalyst exhibits outstanding operational stability, maintaining performance for over 12 hours with minimal degradation. These findings demonstrate the viability of this engineered nanostructure as a promising and cost-effective alternative to commercial benchmark OER electrocatalysts.

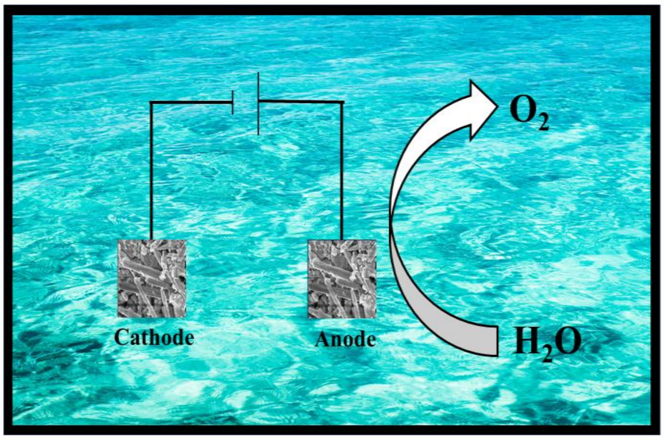

Figure 1. Graphical abstract

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Hydrodeoxygenation of Glycerol to Propene Over Molybdenum and Niobium Phosphate Catalysts

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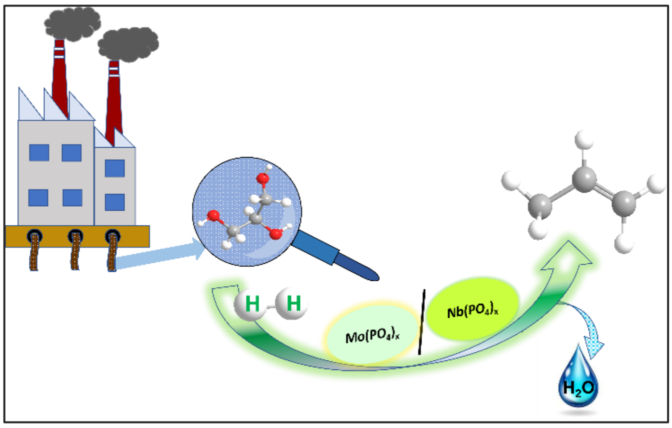
In the single-step conversion of glycerol to propene, the complex catalytic pathway using molybdenum and niobium catalysts are still not well understood. These catalysts can perform the hydrogenolytic cleavage of the glycerol CO bonds efficiently, resulting in a good selectivity of propene. This study explores the reaction routes along with the role of hydrogen plays in product distribution. The hydrodeoxygenation (HDO) of glycerol was investigated using various glycerol purities like raw (purity 80%), technical (purity 85%), and pure glycerol. $Nb(PO_4)_x$ catalyst performs well in batch operation with raw glycerol, indicating that impurities had no detrimental effect on the catalyst's activity. Also in batch mode, $Mo(PO_4)_x$ catalyst achieves a propene selectivity around 50% along with a complete conversion of glycerol at 573 K and 30 bar H_2. In continuous operation, $Nb(PO_4)_x$ achieves highest product selectivity to propene (12%) at low temperatures (573 K), while more C_2 to C_6 alkanes were formed at increased temperatures (623 and 673 K). The production of C_2 to C_6 alkanes and alkenes vary in an opposing manner with temperature. H_2 atmosphere leads the reaction pathway towards the formation of propene and other hydrocarbons via different routes. A balanced presence of both acidic site and metal site provides suitable environment for dehydration and hydrogenation respectively. Both catalysts are characterized using Powder XRD, XPS, Py-IR, N_2 physisorption, NH_3-TPD, SEM and solid state ^{31}P- NMR. This work has elucidated new routes to upcycle bio-renewable glycerol to propene over $Mo(PO_4)_x$ and $Nb(PO_4)_x$ catalysts.



Scheme 1. Hydrodeoxygenation of glycerol to propene over $Mo(PO_4)_x$ and $Mo(PO_4)_x$ catalysts.

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Synthesis and Characterization of Dioxidovanadium(V) Complexes of Dibasic Tridentate Arylhydrazone Ligands for the Selective Epoxidation of Olefins by Hydrogen Peroxide-Assisted Bicarbonate

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Arylhydrazone ligands Hsal-bzh (I), Hcsal-bzh (II), Hbsal-bzh (III), and Hnsal-bzh (IV) were synthesized using ethyl benzoate, hydrazine hydrate, salicylaldehyde and its 5-substituted –Cl, –Br, and $–NO_2$ derivative from refluxing methanol. Carefully characterized ligands I-IV, were reacted with appropriate vanadium precursor to isolate the oxidomethxidovanadium(V) complexes [VO(sal-bzh)(CH_3OH)(OCH_3)] (1), [VO(csal-bzh)(CH_3OH)(OCH_3)] (2), [VO(bsal-bzh)(CH_3OH)(OCH_3)] (3) and [VO(nsal-bzh)(CH_3OH)(OCH_3)] (4) as well as dioxidovanadium(V) complexes K[V^VO_2(sal-bzh)] (5), K[V^VO_2(csal-bzh)] (6), K[V^VO_2(bsal-bzh)] (7) and K[V^VO_2(nsal-bzh)] (8). A few techniques like ^{51}V NMR, ^{1}H NMR, ^{13}C NMR, single crystal X-ray analysis, HR-MS analysis were performed to confirm the molecular structure of the vanadium(V) complexes in solid state as well as in solution. Dioxidovanadium(V) complexes 5–8 show good catalytic performance towards the homogeneous epoxidation of a series of olefins with high TOF values. Electron-rich and sterically accessible olefins indene exhibit the highest substrate conversion (94%) with very high TOF values of 3.032×103 h−1, and the least reactivity is observed in electronically poor allylbenzene. Generally, catalysts with the electron-withdrawing group at the 5-position of salicylaldehyde in 6–8 exhibit marginally better performance than catalysts with unsubstituted salicylaldehyde. During the catalytic reaction, the formation of oxidoperoxymonocarbonatev anadium(V) {[V^VO_2(OCO_3H)(nsal-bzh)]+H} intermediate, which is supposed to be the key component for epoxidation, was identified by ^{51}V NMR and confirm by HR-MS analysis.

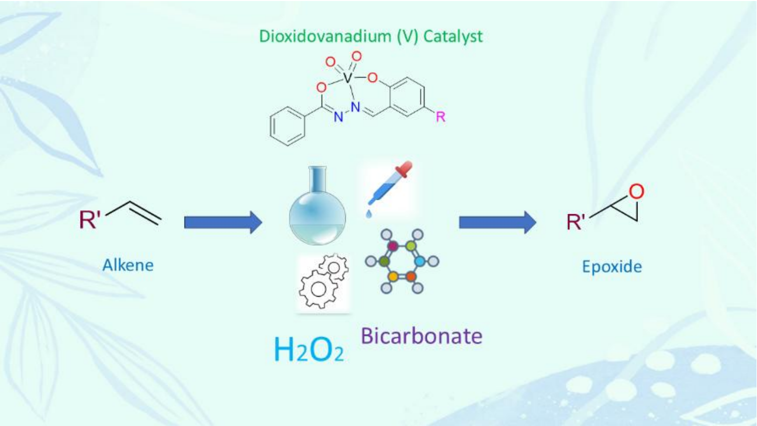

Fig: Graphical abstract for selective epoxidation of olefins by dioxidovanadium(V) species.

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Synthesis, Characterization and Application of Multiwalled Carbon Nanotubes Supported Cobalt Stannate Nanocomposites for Small Molecules Assisted Oxygen Evolution Reaction

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Designing and developing effective bifunctional electrocatalyst is significant in alleviation of global energy conversion and storage devices. In this study bifunctional electrocatalyst were developed using bimetallic oxide and multiwalled carbon nanotubes (MWCNTs) using co-precipitation followed by thermo-mechanical grinding method using varying amount of MWCNTs. The synthesized material's structural and oxidation state were confirmed from X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) analysis. Notably, electrocatalyst have shown increased current density and low overpotential of 190 and 100 mV for oxygen evolution reaction (OER) and methanol oxidation reaction (MOR) at 10 mA/cm^2. Tafel slope for respective OER and MOR were also found to be 75 and 69 mV/dec. Electrocatalyst have also shown significant reduction in charge transfer resistance leading to enhancement in electrode kinetics at interfaces. Substantially material has shown exceptional electrocatalytic activity because of increased surface area and enhanced electrical conductivity due to synergistic effect observed in the synthesized nanocomposites. The materials stability for long term operation was also confirmed from chronoamperometry at given overpotential for 14 and 12 h duration for OER and MOR respectively. The electrocatalyst was also found to be effective at higher concentration of 1M methanol. It has also shown excellent stability as confirmed from chronoamperometry making it effective and efficient alternative electrocatalyst for oxygen evolution reaction via advanced conversion technologies.

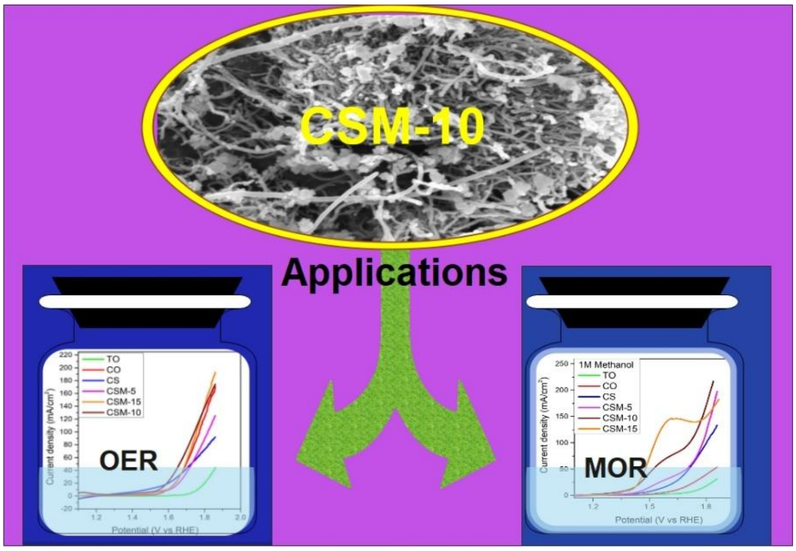

Figure- Graphic representation of nanocomposite and their applications in OER and MOR

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Metal-Dependent Proton Responsiveness in Electrochemical CO_2 Reduction: A Comparative Study of Isostructural Ni(II) and Cu(II) Schiff-Base Complexes

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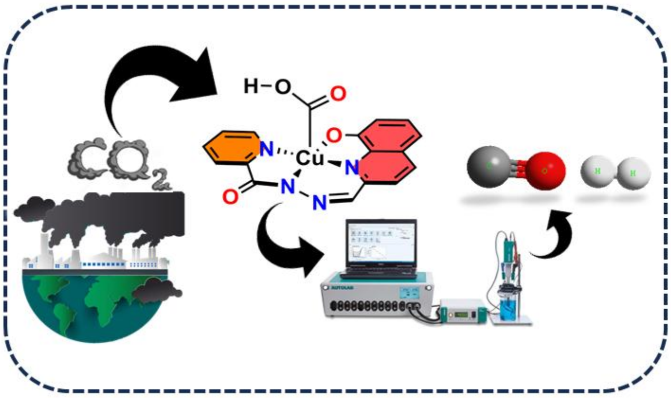
Two mononuclear Ni(II) and Cu(II) Schiff-base complexes supported by the same planar tetradentate ligand were synthesized and investigated as molecular electrocatalysts for CO_2 reduction in DMF medium. Both complexes exhibit nearly identical cyclic voltammograms under argon indicating closely comparable electronic environments imposed by the ligand framework. Electrocatalytic CO_2 reduction was examined under CO_2 atmosphere in the presence of varied proton sources (H_2O, TFE, and phenol). The Cu(II) complex displays strong proton-dependent catalytic activity: addition of water (up to 1 M) or TFE results in large catalytic current enhancements with faradaic efficiencies for CO production exceeding 85% at modest overpotentials. Remarkably, the Ni(II) analogue, despite possessing an almost superimposable redox potential, shows no catalytic response under identical conditions. No current increase is observed even in the presence of excess water, TFE, or phenol, and bulk electrolysis yields CO with less faradaic efficiency. This work reveals a striking metal-dependent switch in proton responsiveness for CO_2 reduction within an otherwise identical ligand framework.



Scheme 1. Comparative CO_2 Reduction using Schiff base electro catalysts.

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Adsorption of hydrogen, methane, and their mixtures on Na-functionalized [1, 1] Paracyclophane: an atomistic investigation

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Abstract

This work presents a computational assessment of sodium-functionalized [1,1] Paracyclophane (PCP11) for onboard storage of hydrogen, methane, and their mixtures under U.S. Department of Energy (DoE)-relevant conditions. The Na–substrate interaction is relatively weak, with a binding energy of 0.635 eV, yet sufficient to enable reversible gas adsorption. Simulations indicate PCP11–Na can host up to 10 H2 and 8 CH4 molecules, as well as mixed H2/CH4 loadings across various compositions, governed by Niu–Rao–Jena polarization-mediated interactions. The average adsorption energies are 0.125 eV per H2 and 0.195 eV per CH4, aligning with physisorption suitable for practical adsorption–desorption. The resulting gravimetric capacities reach 8.18 wt% for hydrogen and 36.19 wt% for methane, satisfying DoE storage benchmarks. Charge polarization and binding mechanisms are elucidated through projected density of states, electrostatic potential mapping, and Hirshfeld charge analyses. Thermodynamic estimates yield average desorption temperatures of 160.27 K for the hydrogenated system and 250.31 K for the methane-loaded system, indicating moderate thermal inputs for release. Atom-Centered Density Matrix Propagation confirms structural integrity and reversible uptake–release cycles without host distortion. Collectively, these results highlight Na-functionalized PCP11 as a lightweight, molecular host that combines adequate metal–substrate binding with reversible multi-molecule adsorption and favourable energetics for hydrogen, methane, and mixed-gas storage within regulatory targets.

Keywords: Hydrogen storage; Methane storage; Paracyclophane; Charge polarization.

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Density Functional Study of Reversible Hydrogen Storage in Sc-decorated [6]cycloparaphenylene

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Abstract

This work explores the hydrogen storage properties of scandium-functionalized [6]cycloparaphenylene ([6]CPP) through dispersion-corrected density functional theory (DFT + D3) calculations. The binding energy of the Sc atom is found to be 1.33 eV. The system can accommodate up to 30 H_2 molecules in a quasi-molecular state, with adsorption energies ranging from 0.23 to 0.36 eV per H_2 molecule. The stability of the system, both prior to and after hydrogen adsorption, is evaluated using reactivity descriptors. At low temperatures and pressures ranging from 1 to 60 bar, the system achieves a maximum gravimetric hydrogen capacity of 7.68 wt%. Above room temperatures, the gravimetric density remains above 5.5 wt%, surpassing the US Department of Energy benchmark, within a pressure range of 1 to 60 bar. Molecular dynamics simulations using Atom-Centered Density Matrix Propagation (ADMP) indicate that hydrogen desorption initiates near 300 K and 1 bar; however, higher temperatures are required for complete desorption. The Van't Hoff temperature is calculated as 296.9 K at 1 atm for the system. Furthermore, the negligible structural variations of [6]CPP–Sc throughout adsorption and desorption highlight its stability and reversibility. Therefore, Sc-decorated [6]CPP shows strong potential as an efficient material for hydrogen storage.

Keywords: Hydrogen storage; DFT; Cycloparaphenylene; ADMP

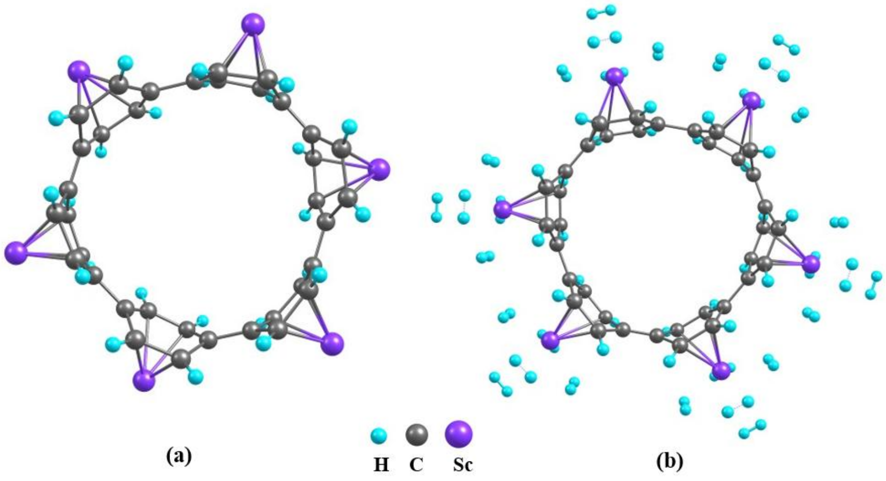

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Photo-Thiocyanoamination of π- and σ-Bonds: Reagent Development and Synthetic Applications

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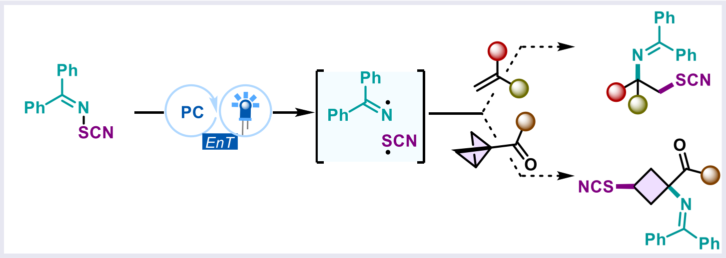
1,2-thiocyanoamines make up a class of important structural motifs that are found in a number of bio-active molecules and precursors to many more. Despite their synthetic significance expedient access to this difunctionalization is rare. Herein, the development of a thiocyanoimination reagent is disclosed, taking advantage of photo-mediated energy transfer phenomena for the facile thiocyanoimination of alkenes. The strategy was found to be viable for σ-bonds as well, providing a generalized strategy for accessing small molecules infused with amine and -SCN.



Scheme 1/Figure: Photocatalytic Thiocyanoamination of olefins

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Band Structure Engineering for Newly Synthesised Transition Metal Carbo-Chalcogenides via Strain, Doping, and Defect: A Density Functional Theory Investigation

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Transition metal carbo-chalcogenides (TMCCs) represent a novel class of two-dimensional materials exhibiting promising electronic, mechanical, and catalytic properties. This study focuses on band structure engineering of TMCCs through systematic computational approaches involving strain application, atomic substitution (doping), and vacancy defects. Using density functional theory (DFT) calculations, we investigate the effects of these modifications on the electronic structure, aiming to tune the bandgap and carrier effective masses for potential device applications. In addition to electronic properties, preliminary efforts are made to explore thermal conductivity and dielectric behavior, critical for developing TMCC-based nanoelectronics and energy devices. In the initial findings no major band structure change has been observed with strain although it is observed that band gap seems to open with vacancy, although material remains metallic as earlier. The results highlight the interplay between structural perturbations and fundamental physical properties, providing insights into defect and strain engineering strategies. This work contributes to closing the computational knowledge gap on TMCCs by combining electronic and transport property analysis, paving the way for rational design of multifunctional 2D materials.

This work is in progress.

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