CHAPTER 14

CHEMISTRY

Doctoral Theses

01. AGARWAL (Archana)
Synergistic Design of Nanomagnetic silica and Ionic Liquid Interfaces as Nanocatalysts for Sustainable Organic Synthesis.
Supervisor: Prof. Subho Mozumdar
Th 28968

Abstract

The development of efficient, reusable, and environmentally friendly catalytic systems is crucial for advancing sustainable organic synthesis. This thesis presents the design, synthesis, characterization and application of novel ionic liquid-based heterogeneous nanostructured materials supported on Nanomagnetic silica cores for organic transformations. It begins with a comprehensive introduction to nanomaterials, emphasizing their unique physicochemical properties, classification, and their transformative role in nanocatalysis. Special focus is given to their ability to enhance catalytic activity, selectivity, and recyclability—addressing critical challenges of conventional homogeneous catalysts. A variety of advanced characterization techniques, including FT-IR, NMR, SEM, TEM, XRD, XPS, BET, TGA, and VSM, were employed to confirm the successful synthesis and understand the structural, thermal, and magnetic properties of the developed nanocatalysts. The core experimental work involved synthesizing two major catalytic systems: an imidazolium-based ionic liquid immobilized on $Fe_3O_4@SiO_2$ nanoparticles and a dicationic DABCO-based ionic liquid anchored on similar magnetic supports. These catalysts were designed to offer high basic site density, excellent thermal and chemical stability, and effortless magnetic recovery. The catalytic activity of the synthesized materials was evaluated through the synthesis of pharmaceutically important heterocyclic compounds such as benzopyran, pyranopyrazole, and polyhydroquinoline derivatives. The reactions proceeded efficiently under mild, solvent-free, or aqueous conditions, yielding high product outputs with short reaction times. Furthermore, the catalysts demonstrated excellent reusability over multiple cycles with negligible activity loss, underscoring their stability and practical utility. This work successfully establishes a greener catalytic platform by integrating the advantages of ionic liquids with magnetically separable nanostructured supports. Beyond organic synthesis, these catalysts hold significant promise for future applications in environmental remediation, gas capture, sensing technologies, and biomedical fields.

Contents

1. Introduction and Literature Review 2. Characterization Techniques 3. Imidazolium based Ionic Liquid Anchored over Dendritic Mesoporous Silica Nanospheres possessing a Magnetic Core as an Efficient and Recyclable Base

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02. ANNAN (Ibrahim)
Development of Coumarin-based Chemosensors for the Detection of Selected Analytes.
Supervisor: Prof. Rajeev Gupta
Th 29383

Abstract

Coumarin is a well-known organic dye widely used by the scientific community to design chemosensors due to its strong and stable emission, high quantum yield, good structural flexibility, and excellent biocompatibility. The fluorescent chemosensors based on the coumarin scaffold have been extensively investigated as they enable monitoring of the targeted analytes under environmental and physiological conditions. The primary objective of this dissertation is to design fluorescent chemosensors based on the coumarin moiety for the detection of selected analytes. The design of these chemosensors has been accomplished in such a manner that they offer a chelating site for binding and recognition purposes, along with a fluorophore for signaling purposes. The photophysical properties and structural versatility of these chemosensors have been thoroughly investigated, and low-cost detection techniques, such as colorimetric methods and filter paper-based test strips, have also been developed. The PhD thesis is divided into five chapters, with Chapter 1 providing a brief overview of coumarin, its photophysical properties, and the selected coumarin-based chemosensors. In chapter 2, two closely related coumarin-based chemosensors, L1 and L2, have been designed as the fluorescent sensors for the selective detection of Mg2+ and Zn2+ ions, respectively. Chapter 3 presents two fluorescent probes, L1 and L2, which have been utilized for the detection of multiple analytes, including an amino acid and cations, via emission 'turn-on' response. In chapter 4, two coumarin-functionalized chemosensors, L1 and L2, have been investigated for their metal-ion detection abilities using emission and absorption spectroscopy. The chemosensors L1 and L2 exhibit selective "turn-on" detection of Hg2+ and Pb2+ ions, respectively. Chapter 5 describes a tricyano-furan-coumarin-based probe L, which is used for the exclusive emission 'turn-on' detection of arginine in water. Probe L also exhibits excellent solvatochromism, while its viscosity-sensitivity allowed assessment of changes in the viscous environment in binary solvent systems.

Contents

1. Introduction to Coumarin, its Photophysical Properties, and the Selected Coumarin-based Chemosensors 2. Substituent Effect on Discriminative Detection of Mg^{2+} and Zn^{2+} Ions by Two Related Coumarinbased Chemosensors 3. Coumarin-naphthalimide-based Fluorescent Probes for the Discriminative Sensing of Multiple Analytes 4. Selective and Discriminative Detection of Mercury and Lead Ions by Two Coumarinfunctionalized Chemosensors 5. A Tricyano-furan-coumarin-based Probe: Solvatochromism, Viscosity Studies, and Detection of Arginine in Water 6. Summary. List of Publications, Conferences and Workshops Attended.

03. DHAMA (Nitanshu)

Development of COF Hybrid Materials for Protein Interaction and Electrochemical Energy Storage Studies.

Supervisor: Prof. Dhanraj T. Masram

Th 29333

Abstract

Covalent Organic Frameworks (COFs) are an emerging class of crystalline porous materials that possess high surface area, tunable pore structures, and versatile functionality. However, their practical applications are often limited by poor electrical conductivity and restricted interaction with biological systems. The present research focuses on the design, synthesis, characterization, and application of carbon-based COF hybrid materials for protein interaction studies and electrochemical energy storage. Initially, carbon-based materials and COFs were synthesized and modified to develop advanced hybrid systems with improved physicochemical properties. A series of materials, including Ni-S-GNR, CC-TAPT-COF, TATF-COF, Ag@COF, Tp-$BDMe_2$/GO, COF@MOF, and Act-COF@MOF, were successfully prepared and characterized using XRD, FTIR, Raman spectroscopy, XPS, FESEM, TEM, BET, and other analytical techniques. Structural characterization confirmed the successful formation of the frameworks and hybrid architectures. The biological performance of the synthesized materials was investigated using model proteins, including hemoglobin and lysozyme. Spectroscopic and biophysical studies revealed stable protein–material interactions with minimal structural perturbation, indicating acceptable biocompatibility. Ag@COF further demonstrated antibacterial activity, highlighting its potential for bio-related applications. To enhance electrochemical performance, COFs were integrated with graphene oxide and metal–organic frameworks to form conductive hybrid systems. Electrochemical studies using cyclic voltammetry, galvanostatic charge–discharge, and electrochemical impedance spectroscopy demonstrated improved charge storage behavior, reduced resistance, enhanced ion transport, and superior cycling stability. The synergistic combination of porous frameworks, conductive networks, and redox-active sites significantly improved the supercapacitor performance of the developed materials. Overall, this work demonstrates that rational hybridization of COFs with carbon and metal-based components is an effective strategy for developing multifunctional materials with promising applications in both biomedical studies and advanced energy storage systems.

Contents

1. Introduction 2. Materials and Characterization Techniques 3. Synthesis and Structural Characterization of Carbonintegrated COF and Hybrid Framework Materials 4. Biological and Biophysical Interaction Studies of Synthesized Materials 5. Electrochemical Performance of COF-based Hybrid Electrodes for Supercapacitor 6. Conclusion and Future Work.

04. DHANKA (Ajit Kumar)

Ceria-Based Nanomaterials for Water Splitting and Degradation of Emerging Contaminants.

Supervisor: Dr. Nityananda Agasti

Th 29384

Abstract

The rapid depletion of fossil fuel resources and increasing environmental pollution have intensified the search for sustainable materials for clean energy generation and environmental remediation. Hydrogen production through electrochemical water splitting and photocatalytic degradation of organic pollutants are considered promising solutions to these global challenges. Electrochemical water splitting involves the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), which require efficient and stable electrocatalysts for practical application. Similarly, photocatalytic degradation offers an environmentally friendly approach for removing persistent pollutants such as antibiotics and pesticides from wastewater. However, the efficiency of these technologies is often limited by the lack of highly active, stable, and cost-effective catalytic materials. Among various semiconductor metal oxides, cerium oxide (CeO2) has attracted considerable attention because of its unique redox behaviour, oxygen storage capacity, chemical stability, and reversible Ce3+/Ce4+ oxidation states. The presence of oxygen vacancies in the CeO2 lattice significantly enhances charge transfer and catalytic activity. Nevertheless, pristine CeO2 suffers from a wide band gap and rapid recombination of photogenerated charge carriers, which restrict its photocatalytic and electrocatalytic performance. To address these limitations, defect engineering through metal and metal oxide incorporation has emerged as an effective strategy to modify its structural and electronic properties. In this thesis, defect-engineered CeO2 nanostructures with varying dopant concentrations were synthesised using a solvothermal method and systematically characterised using PXRD, Raman spectroscopy, FESEM, HRTEM, UV–Visible spectroscopy, DRS, XPS, and EPR analysis. The results confirmed enhanced oxygen vacancy concentration, reduced band gap energy, improved charge transfer, and suppressed electron–hole recombination after doping. The synthesised materials exhibited superior electrocatalytic activity toward HER and OER, along with enhanced photocatalytic degradation of organic pollutants under visible-light irradiation. These improvements were attributed to increased active surface sites, enhanced conductivity, efficient charge separation, and higher generation of reactive oxygen species. Overall, the study highlights the potential of defect-engineered CeO2 nanomaterials as multifunctional catalysts for sustainable energy and environmental applications.

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1. Introduction 2. Experimental Methods and Characterization Techniques 3. Oxygen Vacancies Induced Low Overpotentials of Ag/CeO_2 for Electrocatalytic Evolution of Oxygen and Hydrogen 4. Modulation of Oxygen Vacancies Influences Electrocatalytic Performance of Ni-Doped Ceria for Oxygen and Hydrogen Evolution 5. Harnessing Defects in Ag/CeO_2 for Enhanced Photocatalytic Degradation of Antibiotics in Water 6. Defect-Enriched CuO/CeO_2 Nanostructure: Photocatalytic Degradation of Pesticide in Water 7. Summary and Conclusion. List of Publications, Poster and Oral Presentations Workshops.

05. HUSSEIN (Fatimah Ali)
Mononuclear Metal Complexes as Electrocatalysts for Hydrogen Generation: Design, DFT and Electrochemical Studies.
Supervisor: Prof. Sandeep Kaur
Th 29334

Abstract

The thesis entitled "Mononuclear Metal Complexes as Electrocatalysts for Hydrogen Generation: Design, DFT and Electrochemical Studies" is to be submitted to University of Delhi. This work includes the synthesis, structural characterisation of mononuclear transition metal complexes incorporating Schiff base ligands (N2O2-/N3O2-/NO-type) and Mn complexes using different thiolate and phosphine ligands and their electrocatalytic properties for hydrogen evolution in organic media. The thesis is divided into five chapters. Chapter 1 describes the structural/functional aspects of proton reduction with transition metal Schiff base and mononuclear MnI complexes reported till date as HER electrocatalysts. In Chapter 2 electrocatalysis by reported complexes [Mn(Salen)Cl] 1/[M(Salen)] (M = Co, 2/ Ni, 3/Cu, 4) and [Mn(CH3Salen)Cl] 5/[M(CH3Salen)] (M = Co, 6/Ni, 7/Cu, 8) has been delineated. Stability and catalytic efficiency for the catalysts were 2, 4 > 6 > 7 > 3 > 8 (acetic acid) and 1 > 5 (trifluoroacetic acid). DFT studies provided insight into the metal- vs. ligand-centered redox transitions and hydrogen evolution mechanism for the complexes. Chapter 3 deals with the synthesis and characterization of [Mn(HL3)Cl] 9/ [M(HL3)] (M = Co, 10/Ni, 11/Cu, 12) 2,2′-((azanediylbis(propane-3,1-diyl))bis(azaneylylidene))bis(benzene-1,3-diol) (H3L3)) complexes. Electrocatalytic proton reduction was investigated in the presence of weak acid in acetonitrile. Chapter 4 describes the synthesis and characterization of mononuclear complexes [M(L4/L5)2] (M = Co, 13/15; Cu, 14/16) (3-[(E)-(2-hydroxyphenyl)methan-1-ylideneamino]benzoic acid (HL4)/3-[(E)-(2-hydroxy-5-nitrophenyl)methan-1-ylideneamino]benzoic acid (HL5)). Dinuclear complexes [M2(L4/L5)2(py)4] (M = Co, 17/19; Cu, 18/20) were also obtained during the synthesis. Single-crystal X-ray structures were obtained for complexes 17 and 18. The complexes were further investigated for proton reduction to dihydrogen in acetonitrile. In Chapter 5 mononuclear MnI complexes fac-[(Mn(CO)3(κ2-SN2C7H5)(κ1-PPh2Py))] 21 and fac-[(Mn(CO)3(κ2-S2NC7H4)(κ1-PPh2Py))] 22 were synthesized with 2-mercaptobenzimidazole /2-mercaptobenzothiazole and N-based phosphine (PPh2Py) ligands. The complexes effectively catalyzed electrochemical proton reduction with a turnover frequency (TOF /s-1; O.P., η/V) of 610/1.02 (21) and 615/1.12 (22).

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1. Introduction and Literature Survey 2. New Use of Mononuclear Mn/Co/Ni/Cu-Complexes of Symmetric N_2O_2-type Schiff-Base as Hydrogen Evolving Catalysts 3. Electrochemical Proton Reduction Mediated by N_3O_2Type Schiff-Base Mono-nuclear Mn/Co/Ni/Cu Complexes 4. Synthesis and Electrochemical Studies of NO-Type Schiff-Base Co/Cu Complexes for Proton Reduction 5. Hydrogen Evolving Mono-nuclear Manganese Complexes with Carefully Positioned Pyridine Base Ligands. Summary and Conclusion, List of Publications.

06. MAMTA BAI
Extraction and Characterization of Plant Based Photosensitizers and their Application in Dye-Sensitized Solar Cells (DSSCs).
Supervisor: Prof. Mahaveer Genwa
Th 29335

Abstract

Plants have unique mechanism of photosynthesis to harvest solar energy. Photo sensitizers present in the plants plays an important role in this process. In our research work we extracted various types of photosensitizers/dyes from different plants eg. Neolamarckia cadamba, Tinospora cordifolia (stem, leaf), Allium Cepa peel etc. The extracted photosensitizers/dyes are characterised on various parameters like pH, conductivity and UV- visible spectroscopy, XRD. These dyes were used in indigenously fabricate Dye Sensitized Solar Cell (DSSCS).

Contents

1. Introduction 2. Experimental Methods and Characterization Techniques 3. Harnessing Nature's Green Gold from *Tinospora cordifolia* for Sustainable and EcoFriendly Future Dye-Sensitized Solar Cells 4. Design and Performance Evaluation of EcoFriendly Dye-Sensitized Solar Cells Using *Tinospora cordifolia* Stem and *Allium cepa* Peel 5. Sustainable Solar Energy Harvesting by *Neolamarckia cadamba* Leaf Extract and Comparative Study of Solvent Effect on Cell Performance 6. Summary and Future Aspects. List of Publications, Conferences and workshops.

07. MEENA (Mahendra Kumar)
Computational Evaluation of Oxa-/ Thia-azolidines as Potential Inhibitors of nsp2 and nsp3 of Chikungunya Virus: A Molecular Docking and Dynamic Simulation Approach.
Supervisor: Prof. Prashant Singh
Th 28970

Abstract

Chikungunya is an infectious disease caused by the Chikungunya Virus (CHIKV). CHIKV is a positive single stranded RNA virus that belongs to the genus Alphavirus of the Togaviridae family. Both nsP2 and nsP3 proteins have an important role in viral replication and transcription processes. Both nsP2 and nsP3 proteins have an important role in viral replication and transcription processes. The crystal structures of nsP2 and nsP3 were downloaded from the Protein Data Bank with PDB IDs 3TRK and 3GPO respectively. MD simulation of proteins were done for 100 ns at three different temperatures 300 K, 325 K and 350 K in order to study how temperature affects their structural dynamics. Biologically active thiazolidine based compounds was designed and screened against nsP3 and to evaluate their stability and interaction behaviour using computational method. CMPD474 was come out as the most promising inhibitor with a binding energy of −115.94. CMPD474 interacted with important amino acid residues such as TRP150 and ARG146 through π interactions while residues TYR144, LEU110, GLY114, ARG146, CYS145 and THR113 involved in hydrogen bonding interactions. The change in free energy (ΔG) for the complex formation at 300 K was found to be -7.0524 kcal/mol confirms that the formation of the complex was thermodynamically feasible and energetically favourable through MM/GBSA binding free energy calculations(MM/GBSA). A library of 2000 compounds was prepared by changing different substituents attached to the aromatic ring and alkyl nitrile groups. CMPD222 showed the best interaction with nsP2 having

binding energy of -106.999 kcal/mol using the iGEMDOCK. Detailed interaction analysis showed that CMPD222 interacted with important amino acid residues present in the active region of nsP2 such as ASP33, VAL35, TYR144 and ARG146.

Contents

1. Introduction and Literature Review 2. Aim and Objectives 3. Impact of Temperature on structural changes in nsP2 and nsP3 of CHIKV: Molecular dynamics simulation 4. Thiazolidines: An arsenal for the inhibition of nsP3 of CHIKV using molecular docking and MD simulations 5. Promising inhibitors of nsP2 of CHIKV using Molecular docking and temperature dependant Molecular dynamics simulations 6. Summary. List of Papers Published. List of work presented in Conferences.

08. MEENA (Harshvardhan)
In Silico Designing of New Reduced Coumarin Based Anticoagulants and Enhancement of Their Aqueous Solubility.
Supervisor: Prof. Prashant Singh
Th 29336

Abstract

The current study focuses on the computational design and evaluation of new anticoagulant compounds based on reduced coumarins and curcumin derivatives that target human coagulation Factor XA. Molecular docking was employed to determine binding affinity, followed by molecular dynamics simulations with GROMACS and AMBER to examine structural stability and interaction behavior. CMPD227 had high binding affinity and stable interaction with Factor XA. Density Functional Theory (DFT) calculations confirmed its electronic stability. Beta-lactoglobulin (BLG) was explored as a biocompatible protein carrier to enhance the solubility of hydrophobic compounds. CMPD226 demonstrated strong binding with BLG suggesting improved solubility potential. Consistent binding behavior with various biological targets provides a strong scientific basis to investigate curcumin as a potential inhibitor of Factor XA. Curcumin derivatives were also tested as natural anti-coagulants and Curcumin 5 showed promising binding and pharmacokinetic properties. Moreover, Warfarin and Direct anti-coagulant drugs complexation with Beta-lactoglobulin showed edoxaban –BLG complex as the most stable. DFT calculation of Warfarin and DOACs with Methionine evaluated Edoxaban shows the highest electronic stability. This study highlights the potential of reduced coumarins and protein complexation delivery systems in the development of effective and water-soluble drugs.

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1. Introduction and Literature Review 2. Objectives and Methedology 3. Unraveling the Potential of Reduced Coumarins as Anticoagulating Agents via Targeting Human Coagulation Factor XA *In-Silico* Approach 4. Insights into the Interactions Between Bovine β- Lactoglobulin and Reduced Coumarins: A Computational Perspective on Solubility Enhancemant 5. Computational Investigation of Cureumin-Factor Xa Interactions: A Novel Approach to Safer Anticogulants 6. An Insight for the interaction of Warfarin and DOACs with βLactoglobulin to improve the Solubility 7. Summary. List of Publications and Work Presented in Conferences.

09. MOHD SHAKIR

Synthesis of 4-Aminoquinoline Based Molecular Hybrids and their Biological Activity Evaluation.

Supervisors: Prof. Diwan S. Rawat, Prof. Mahendra Nath and Prof. Mohammad Abid

Th 28971

Abstract

The present research work aimed to develop novel drug molecules against serious illnesses affecting humans. Bacterial infections, malaria, and cancers together account for a high rate of morbidity and mortality all over the world. The problem of drug resistance is associated with the treatment of all these diseases. Therefore, there is an urgent need to develop novel drug candidates. They exhibit a wide range of therapeutic effects, such as antimicrobial, antiviral, anti-inflammatory, antidiabetic, antihypertensive, and anticonvulsant activities. Quinoline is one of the most important N-heteroarenes based on its diverse applications in chemical, medicinal, and industrial fields. In particular, 4-aminoquinoline represents one of the most important scaffolds in medicinal chemistry due to its broad spectrum of biological activities. Several 4-aminoquinoline-based drugs are available in the market, such as chloroquine, hydroxychloroquine, piperaquine, and amodiaquine, as antimalarials. Other prominent examples include neratinib and pelitinib as anticancer agents. Chapter 1, “Synthesis and mechanistic studies of 4-Aminoquinoline-Isatin molecular hybrids and Schiff`s bases as promising antimicrobial agents", presents the creation of 7-chloro-4-aminoquinolineisatin-based molecular hybrids (SB1-12) and the creation of 7-chloro-4-aminoquinoline-Schiff`s base compounds (LT-SBI-23). The compounds LT-SB5, 7, and 23 were found to exhibit antibacterial activity. LTSB-7 was found to be effective with an MIC of 64 µg/ml and non-haemolytic. Chapter 2, titled “Design and synthesis of 4-aminoquinoline-tethered natural alcohols connected through 1,2,3-triazole as promising chemotherapeutic agents inhibiting bacterial biofilm", deals with the synthesis and characterisation of 14 natural alcohols hybridised with 4-aminoquinoline by using the 1,2,3-triazole moiety. The compound NA-2 was found to have promising antibacterial activity and non-haemolytic activity. Chapter 3, titled “Design and synthesis of 4-aminoquinoline-substituted pyrazole-based molecular hybrids as antibacterial agents", involved the synthesis of 18 compounds, out of which 2 compounds, 12b and 12c, displayed good antibacterial activity. In chapter 4 titled “Development of potent 4-aminoquinoline-cinnamoyl hybrid antimalarials with structural optimisation, mechanistic insights and biological evaluation”, compounds were synthesised, and out of them, 2 compounds, PC-5 and PC-11, displayed antiplasmodial activity against both chloroquine-sensitive and resistant strains.

Contents

1. 4-aminoquinoline-isatin hybrids and Schiff's bases as antimicrobial agents: Synthesis, mechanistic, and computational studies 2. Designing 4-aminoquinoline-tethered natural alcohols linked via 1,2,3-triazole as promising chemotherapeutic agents to inhibit bacterial biofilms 3. Synthesis and characterisation of regioisomers of quinolinepyrazole molecular hybrids as promising antibacterial agents 4. Development of Potent 4-

Aminoquinoline Cinnamoyl Hybrids as Antimalarials with Structural Optimization, Mechanistic Insights, and Biological Evaluation. Summary, List of Publications and List of Conferences.

10. MOHIT
Design Synthesis and Structural Diversification of Bioactive Molecular Frameworks Curcumin Derived Hybrids and Fused Heterocyclic Systems.
Supervisors: Prof. Diwan Singh Rawat and Prof. Mahendra Nath
Th 29413

Abstract

Synthetic methodologies targeting biologically relevant, highly functionalized heterocyclic scaffolds under mild and sustainable conditions remain a key pursuit in medicinal chemistry. Herein, we report three efficient metal-free strategies for the construction of diverse bio-inspired architectures. First, novel curcumin-based triazine, pyrimidine, and pyrazine hybrids incorporating morpholine, piperidine, and pyrrolidine moieties were designed and synthesized via nucleophilic substitution and Claisen-Schmidt condensation. Secondly, a metal-free, additive-free annulative isocyanide-based multicomponent protocol was developed for the one-pot assembly of novel fused furo[3,2-c] coumarin-pyrazines from 4-hydroxycoumarins, pyrazine-2-aldehydes, and isocyanides. This cascade generates multiple carbon-heteroatom bonds under mild thermal conditions, demonstrating gram-scale applicability, and options for post-synthetic core modification. Finally, a transition-metal- and oxidant-free O-H insertion methodology using aryldiazoacetates and (hetero)carboxylic acids was established for the site-selective synthesis of α-carbonyloxy esters. This protocol displays exceptional chemoselectivity for O-H functionalization in the presence of competing N-H and active C-H bonds across a wide range of complex heterocycles including indole, pyrimidine, and thiazole frameworks. Together, these methodologies expand the toolkit for constructing privileged hybrid frameworks relevant to drug discovery. All the derivatives, obtained in moderate to excellent yields, were characterized using NMR, HRMS, and single crystal X-ray diffraction (SC-XRD).

Contents

1. Introduction to curcumin-based heterocyclic molecular hybrids: Chemistry, biological significance, and therapeutic potential 2A. Synthesis of structurally diverse C5 curcuminoid-triazine molecular hybrids 2B. Heterocyclic remodeling of curcumin: Design and synthesis of C5 curcuminoid-pyrimidine and pyrazine hybrids 3. Catalyst-free one-pot synthesis of novel furo[3,2-c] coumarinpyrazine hybrids *via* isocyanide-mediated multicomponent annulation and in silico evaluation 4. Metal-free O-H insertion enabled access to heterocycle-rich αcarbonyloxy esters. Summary. List of Publications, Seminars and Conferences.

11. MUSKAN
Regio- and Stereoselective Transformation of Alkynes for the Construction of Structurally Diverse Cyclic Frameworks.
Supervisor: Prof. Akhilesh Kumar Verma
Th 28972

Abstract

Regio- and stereoselective construction of cyclic frameworks remains a central challenge in organic synthesis owing to their widespread presence in biologically active molecules and functional materials. Alkynes, due to their versatile reactivity and ability to participate in cascade processes, serve as powerful building blocks for the rapid generation of molecular complexity. The present work focuses on the development of selective alkyne-based transformations employing o-alkynyl carbonyl derivatives for the construction of structurally diverse carbocyclic and heterocyclic frameworks. A series of regioselective annulation and cascade strategies has been developed to access isoquinolone, naphthyridinone, benzofulvene, and indene derivatives under mild and operationally simple conditions. Environmentally benign and atom-economical protocols are established using iodine-mediated cyclizations and one-pot transformations. Selective control over competing cyclization pathways is achieved through Conia-ene spiroannulation and trichloromethylative transformations of o-alkynyl aldehydes. In addition, radical-mediated vinyl radical addition to ketones enables efficient flavanol synthesis, while an unexpected iodine-mediated intermolecular dimerization provides access to symmetrical biaryl ethers. Overall, the work highlights efficient, regio- and stereoselective strategies for alkyne functionalization, offering mechanistic insight and practical routes to structurally diverse cyclic architectures of synthetic significance.

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1A. *o*-Alkynylaryl-2-cyanoacrylates: A Synthon for the Construction of Diverse Isoquinolones /Napthyridinones 1B. Environmentally Benign and Atom-Economical Protocol for the Regioselective Synthesis of Isoquinolones from o-Alkynylaldehydes 2A. Molecular-Iodine-Mediated One-Pot Sequential Iodocyclization-Decarboxylative Protodeiodination: Access to Densely Functionalized Benzofulvenes 2B. Stereoselective Synthesis of Functionalized Indenes *via* Regioselective Cascade Iodoalkylation of Alkynes 3A. Conia-Ene Cyclization of Pyrazolones with o-Alkynyl Aldehydes: A Strategic Shift from Classical Condensation to Spiroannulation 3B. Selective Control of Competing Cyclization Pathways in Trichloromethylative Transformations of o-Alkynyl Aldehydes 4. Unveiling a Long-Elusive Radical Coupling: Flavanol Synthesis *via* Vinyl Radical Addition to Ketones 5. Serendipitous Discovery of Symmetrical Biaryl Ethers via Iodine-Mediated Intermolecular Dimerization of o-Alkynyl Aldehydes. Summary of the Work and Copies of the Publications.

12. NAMRATA

Design and Development of Functionalized Hexagonal Boron Nitride Based Hybrid Electrode Materials for Improved Energy Density Supercapacitors.

Supervisor: Prof. Raj Kishore Sharma

Th 28973

Abstract

The increasing demand for efficient and sustainable energy storage systems has intensified research on advanced electrochemical energy storage devices. Among these, supercapacitors have emerged as promising candidates due to

their high-power density, rapid charge-discharge capability, and long cycling life. However, their relatively low energy density compared to batteries remains a significant limitation. This thesis focuses on the design and development of functionalized hexagonal boron nitride (hBN) based hybrid electrode materials for high-performance supercapacitors with improved energy density. Although hBN possesses excellent chemical stability, thermal stability, and mechanical strength, its wide band gap and poor electrical conductivity restrict its direct application in electrochemical energy storage. To address these limitations, various strategies such as exfoliation, functionalization, porosity engineering, and composite formation have been employed. In this work, bulk hBN was exfoliated into two-dimensional nanosheets to increase the available surface area and expose more electrochemically active sites. Surface functionalization using -OH and -NH groups was carried out to improve electrolyte wettability and facilitate efficient charge transfer. Furthermore, hybrid composites were developed by integrating functionalized hBN with electroactive materials such as α-cobalt hydroxide and carbon dots, resulting in enhanced electrical conductivity and improved ion transport pathways. The results demonstrate that the hybrid electrode materials exhibit significantly improved electrochemical performance compared to pristine hBN. In particular, the functionalized hBN/α-$Co(OH)_2$ composite forms a p-n heterojunction that enhances charge transfer and delivers high specific capacitance and energy density. Additionally, the porous S-hBN@CD structure provides efficient ion diffusion and a large electroactive surface area. The symmetric supercapacitor device shows stable operation at an extended voltage window and excellent cycling stability. Overall, this study demonstrates that functionalization and hybridization of hBN-based materials provide an effective strategy for developing advanced electrode materials for next-generation high-energy supercapacitors.

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1. Introduction 2. Characterization Techniques 3. Fabrication of α-$Co(OH)_2$@f-hBN Composite Based Aqueous Supercapacitor with Wide Operating Potential Window 4. Surfactant-Assisted Exfoliation of hBN and Carbon Dot-Induced Porosity for High-Performance Supercapacitor Electrodes 5. Conclusion. Paper Published & Conference.

13. PRIYANKA

Exploring Metal-Organic Framework-Based Materials: Designing, Fabrication and Their Catalytic Potential in Multicomponent Reactions.

Supervisors: Prof. Anju Srivastava and Dr. R. K. Sharma

Th 28975

Abstract

Metal-organic frameworks (MOFs), also known as class of porous crystalline materials that are composed by linking organic ligands with metal ions/clusters. Due to the unique properties, MOFs has been extensively utilized in variety of applications such as, catalysis, gas storage, sensing, magnetism, drug delivery, energy storage etc. Despite the exceptional properties of MOFs, it suffers several limitations such as thermal instability, chemical degradation in the presence of moisture, acids, or bases and mechanical fragility limiting their use in high temperature and pressure conditions. To address these challenges, MOFs have been proven to be ideal sacrificial templates for fabricating nanoporous carbon,

nanostructured metal oxides, and carbon–metal hybrid materials via MOF mediated synthesis, leading to enhanced stability while retaining the advantages of MOFs. The incorporation of magnetic nanoparticles into MOF structures offers a synergistic effect, significantly improving catalytic performance by increasing stability, surface area, and accessibility of active sites. Moreover, the high saturation magnetization of these composite materials allows for rapid and effortless separation under an external magnetic field, providing a sustainable and cost-effective alternative to conventional separation methods such as filtration and centrifugation. In industrial and environmental catalysis, where recyclability and reusability of catalytic materials are crucial, magnetic MOF composites emerge as a promising solution to enhance both economic feasibility and environmental sustainability. Inspired by the remarkable features of these hybrid materials, we have successfully synthesized and characterized a series of MOF-derived metal oxides nanoparticles, MOF-magnetic composites, and MOF-graphene oxide composite, and investigated their catalytic performance in various industrially and pharmaceutically significant organic reactions. Specifically, these advanced catalysts proved highly effective in the multicomponent synthesis of 2,3-dihydroquinazoline, 5-substituted imidazole, and 1-[((5-methylbenzo[d]thiazol-2-yl)amino)(aryl)methyl)] naphthalen-2-ol derivatives, highlighting their broad applicability and robust catalytic efficiency. The development of such functional materials not only advances the field of MOF-based catalysis but also paves the way for designing highly efficient, recyclable, and industrially viable catalytic systems.

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1. Introduction 2. Theoretical Aspects of Analytical Techniques Employed for Physico-Chemical Characterizations 3. Unleashing the Catalytic Potency of Nanoporous Copper Oxide Particles Derived from Copper 5-Nitroisophthalate MOF towards the Multicomponent Synthesis of 2,3-Dihydroquinazolinones 4. Unexplored Catalytic Potency of a Magnetic $CoFe_2O_4$/Ni- BDC MOF Composite for the One-Pot Sustainable Synthesis of 5- Substituted *1-H* Tetrazoles 5. Magnetic $CoFe_2O_4$ Nanoparticles on Mn-BTC MOF for Applications as Catalysts for Multicomponent Syntheses 6. Design and Fabrication of a Co-MOF@GO-Based Heterogeneous Catalyst for the Morita-Baylis-Hillman Reaction. Summary, Research Publications, List of International and National Conferences Attended.

14. RAGUI (Pamthingla)

Synthesis and Characterization of Multi-Metallic Metal-Organic Frameworks and Nanocomposites for Environmental Remediation.

Supervisors: Prof. Rakesh Kumar Sharma and Dr. Vijay Kumar

Th 28977

Abstract

Chapter 1 outlines the broad introduction and current progress in MOFs and nanocomposites. The behavior of MOFs and nanocomposites with multi-metals are discussed in this chapter. Further, it explored the presence of various Organic Contaminants in water and its impact on human health and environment in general. Chapter 2 mainly focuses on the techniques that have been employed for the characterization of prepared materials to study adsorption mechanism. Also, the study of the process of adsorption or removal of OCs on the synthesized materials were done using UV-Vis

spectroscopy by monitoring the change in the absorbance value of OCs which were observed with respect to the λmax of the respective OCs. Chapter 3 discussed the synthesis, and characterization of bimetallic MOFs, F:N@BTC using Iron-Nickel metal ions and 1,3,5-benzenetricarboxylic acid as organic linkers along with its monometallic counterparts F@BTC and N@BTC. The MOFs were investigated for the removal of Organic Contaminants (OCs), antibiotics and dyes (CF, NA, TB, RB, and RoB). Chapter 4 discussed the synthesis, and characterization of trimetallic metal-organic frameworks, FNC@BTC. The synthesized MOFs was further used for the removal of antibiotics in water. Chapter 5 explored the synthesis, and Characterization of Ti based MXenes, Ti3C2Tx from its MAX phase. Ag and Ni are loaded on the MXene to synthesize nanocomposite, AgNi@MXene. Further, AgNi@MXene nanocomposite was employed for the removal of dye, methylene Blue (MB). Chapter 6 concludes that the study of this thesis investigates the synthesis of multi-metallic MOFs (F:N@BTC, FNC@BTC) and MXene nanocomposite (AgNi@MXene) and optimized by characterizing using various characterization techniques. The efficacy of synthesized multi-metallic MOFs and MXene nanocomposite as functional materials for the adsorptive and catalytic elimination of OCs from water exhibits outstanding activity, addressing a critical need for environment remediation.

Contents

1. Introduction and Literature Survey 2. Characterization Techniques 3. Bimetallic MOFs for the Effective Removal of Organic Contaminants: Dyes and Antibiotics 4. Trimetallic FeNiCo@BTC Metal-Organic Frameworks for the Effective Removal of Antibiotic: Ciprofloxacin 5. Synthesis of AgNi@Mxene Nanocomposite for the Degradation of Dye: Methylene Blue 6. Conclusion. List of Publications. List of International and National Conferences.

15. RAO (Shivangi)
Evaluation of physical and electrochemical properties of a few modified 2D-, and 3D-oxides and 2Doxychlorides.
Supervisor: Prof. Rajamani Nagarajan
Th 28978

Abstract

Investigating relation between the structure and the properties of materials is critical for optimizing existing materials and creating novel ones for specific applications. Structure-property correlation is the foundation for “materials by design”. It allows researchers to intentionally modify the structure, such as altering the atomic arrangement, chemical composition, or intermolecular forces, to achieve desired properties. With this objective, the current thesis aims to investigate the structure-property relationships of technologically important oxides and oxychlorides. The physical properties include dielectric, ferroelectric, magnetic, and electrochemical. A succinct introduction on how the structure and property are interrelated in Bi2O3, perovskite-structured ABO3, triple fluorite containing Sillen type Bi2GdO4Cl, Bi2YO4Cl and CaBiO2Cl, is provided in Chapter 1. Research work related to reversible iodine intercalation in quasi-2D rhombohedral Bi0.775Ln0.225O1.5 (Ln = La, Nd, Sm, and Eu) and their use as anode material in lithium-ion batteries is discussed in Chapter 2. The work on the effect of cationic substitutions at the Pr- and Fe-sites of PrFeO3 on its dielectric, ferroelectric and magnetic properties is covered. Interesting magnetic interactions, including a spin-

reorientation transition and a negative exchange bias effect, were observed in PrFeO3 samples with Bi3+ substituting for Pr. Magnetic frustration due to competing ferromagnetic and antiferromagnetic interactions was evident at low temperature in PrFeO3 samples magnetically diluted with Ga and In at the Fe site. An intricate analysis of inverse magnetic susceptibility measurements revealed the emergence of a Griffiths-like phase (GP). The structure, optical, magnetic, and dielectric/ferroelectric properties of PrFeO3 synergistically co-substituted Bi3+ and Al3+ have been presented. In Chapter 4, research work dealing with triple fluorite containing Sillen type Bi2GdO4Cl, Bi2YO4Cl and CaBiO2Cl, a member of the Sillen X1 family of bismuth-containing oxychloride are described. The overall outcomes and their implications to design technologically important solids are compiled in the concluding section.

Contents

1. Introduction 2. Work related to 2D-oxides and their iodine intercalated analogues, and evaluation of their electrochemical studies 3. Work on 3D-oxide: Exploring multifunctionality of $PrFeO_3$ 4. Work on 2D-oxychlorides: Bismuth containing oxychlorides of the Sillen X1 family. Conclusions and future directions. List of publications, conferences, and workshops attended.

16. SANJAY
Tuning the Phase Transition of Thermoresponsive Polymers via Nanoparticles Modified with Ionic Liquids and Deep Eutectic Solvents.
Supervisor: Prof. P. Venkatesu
Th 28981

Abstract

Advancements in the field of polymer science have resulted in the development of a novel class of polymers called stimuli-responsive polymers (SRPs) or smart/intelligent polymers. These polymers can reversibly adjust their physical and/or chemical properties in response to external stimuli such as-temperature, light, and pH, mechanical force, ultrasound, the presence of different small molecules etc. Among these, thermoresponsive polymers (TRPs) have garnered widespread scientific interest because of the coil-to-globule phase transition. Some of extensively studied TRPs are poly(N-vinylcaprolactam) (PVCL), poly(vinyl methyl ether) (PVME), and poly(N-isopropylacrylamide) (PNIPAM). A common feature of all these polymers is lower critical solution temperature (LCST) around ~30 – 36 °C, which is remarkable close to the physiological temperature. Within this temperature range, the polymer chains are hydrated and expanded; however, above the LCST, dehydration leads to collapse of polymer chains, leading to release of encapsulated molecules. These reversible transitions, combined with biocompatibility and structural tunability, make TRPs promising candidates for controlled and targeted drug delivery systems. Among various TRPs, diblock copolymer poly(N-isopropylacrylamide)-b-poly(acryloylmorpholine) (PNIPAM-b-PACMO), triblock copolymer, poly (ethylene glycol)-block-poly (propylene glycol)-block-poly (ethylene glycol) (PEG-PPG-PEG), diblock copolymers poly(N-acryloylmorpholine)-b-poly(N-isopropylacrylamide) (PACMO-b-PNIPAM) are considered in the present work. Nanomaterials are classical candidates to improvise macromolecules with fascinating physical properties. Numerous chemical and physical properties

of metal nanoparticles (NPs) have made them the subject of intensive research. In particular, gold nanoparticles (AuNPs) and silver nanoparticles (AgNPs) are employed in many fields such as biosensing, catalysis, electronics, therapeutic agents and cancer therapy among others. AuNPs and AgNPs have their nanosize and large surface to mass ratios which contribute towards the interaction of nanoparticles with macromolecules. The biocompatibility of AuNPs and AgNPs with macromolecules is a key factor in proposing their various bio-applications.

Contents

1. Introduction and Review of the Lirerature 2. Materials and Experimental Techniques 3. Influence of Ionic Liquid Modified Gold Nanoparticles on Conformational Transition of Poly (N-Isopropylacrylamide)-b-Poly(Acryloylmorpholine) Block Copolymer 4. Conformational Analysis of Temperature Switchable PNIPAM-b-PACMO in Ionic Liquid Modified AuNPs: A Comprehensive Insight into Nanocomposites Formation-Phase Transition Relationship 5. Alteration of Hydrophilic/Hydrophobic Balance of Triblock Copolymer: A Nanocomposite Bridge Formation between PEG-PPG-PEG and AgNPs Coated with DESs 6. Modulation of hydrophilic-hydrophobic balance in PACMO-b-PNIPAM using deep eutectic solvent modified magnetic nanoparticles 7. Conclusions. Publications.

17. SINGH (Jugmendra)
Design and Synthesis of Indole Derived Schiff's Base Ligands and their Metal Complexes for Biological and Catalytic Applications.
Supervisor: Dr. Umesh Kumar
Th 28982

Abstract

The present thesis is divided into five chapters. The first chapter of the thesis provides a general introduction and objectives of this work. In chapter 2, we have synthesized and characterized indole-based ligand (L2.1) and its Fe(III) (2.1), Co(II) (2.2), Ni(II) (2.3), and Cu(II) (2.4) complexes. In vitro antimicrobial studies of ligand and metal complexes were assayed against various pathogens. Complexes 2.1 and 2.2 exhibited better antifungal and antibacterial, respectively for examined pathogens. In chapter 3, we have synthesized and characterized indole-based CNP donor ligand [PhCH2-(NC8H5)-CH=N-(C6H4)-2-P(Ph)2](L3.1) and its palladium complexes [(μ-CNP-L3.1-H)-Pd-Cl] (3.1) and [(μ-NP-L3.1)-Pd-Cl2] (3.2). The cytotoxicity of L3.1, 3.1, and 3.2 has been evaluated against 4T1 breast cancer cells. The lower half-maximal inhibitory concentration value (IC_{50} = 25.6 μM) of complex 3.1 compared to 3.2 (IC_{50} = 30.1 μM) and the standard drug cisplatin (IC_{50} = 26 μM) indicates that complex 3.1 shows better cytotoxicity than 3.2 and cisplatin. In chapter 4, we have synthesized and characterized indole-based CNS donor ligand [PhCH2-(NC8H5)-CH=N-(C6H4)-SCH3)] (L4.1) and its Pd (II) complexes [(μ-C(ortho)NS-L4.1-H)-Pd-Cl] (4.1) and [(μ-C(peri)NS-L4.1-H)-Pd-Cl] (4.2). The ORR electrocatalytic activities of complexes 4.1 and 4.2 were evaluated in O_2-saturated 0.1 M KOH solution. Complex 4.1 exhibited a lower onset potential (-0.11V) and higher current density (-0.28 mA cm^{-2}) compared to complex 4.2, indicating its superior catalytic performance. In chapter 5, we have synthesized and characterized indole-based novel CNS donor ligand [PhCH2-(NC8H5)-CH=N-(C6H4)-SPh)]

(L5.1) and its Pd complex [(μ-CNS-L5.1-H)-Pd-Cl] (5.1). The ORR electrocatalytic activity of complex 5.1 was evaluated in O_2-saturated 0.1 M KOH solution which exhibited low onset potential (-0.12 V) and high current density (-0.15mA cm^{-2}) indicating its promising catalytic performance.

Contents

1. Introduction of the present investigation 2. Indole-based Schiff's base ligated transition metal complexes: Synthesis, and characterization, computational, and antimicrobial studies 3. Bioinspired indole-based CNP donor ligand and its Pd(II) complexes: Synthesis, and characterization, computational, and *in vitro* cytotoxicity against breast cancer 4T1 cells 4. Indole based CNS donor ligand and its *ortho*- and *peri*-cyclopalladate: Synthesis, and characterization, computational, and electrochemical oxygen reduction reaction studies 5. Palladacycle bearing indole derived CNS donor ligand: Synthesis, and characterization, computational, and electrochemical oxygen reduction reaction studies. Appendix-I (Supporting information's). List of new compounds synthesised in the present investigation. Summary. Synopsis. List of Publications and Conferences.