CHAPTER 9

CHEMISTRY

Doctoral Theses

01. AALAM (Mohd. Jubair)
Development of Reusable Organocatalysts for the Asymmetric Diels-Alder and Friedel-Crafts Reactions.
Supervisor: Prof. Surender Singh
Th 26579

Abstract

The thesis reveals the synthesis of chiral organocatalysts such as modified MacMillan organocatalyst, chiral imidazolidinone and these chiral organocatalysts were applied in different organic transformations such as asymmetric Diels-Alder, and enantioselective Friedel-Crafts reactions. Chapter 1:General Introduction to Chirality and Asymmetric Diels-Alder and Friedel-Crafts Reactions**.** Chapter 1 deals with the introduction to the asymmetric synthesis carried by organocatalysis, metal catalysis, and biocatalysis. It also includes the historical background of chirality and its importance in *day* to day life. Chirality has the most significance in living life because of the higher functionality of one of its pure enantiomeric forms. Pure chiral compounds were effectively used in different areas such as agrochemicals, fragrances and flavors, vitamins and pharmaceuticals, and many others. This chapter also comprises the literature survey of asymmetric Diels-Alder and Friedel-Crafts reactions. Chapter 2: Chiral Imidazolidin-4-one with Catalytic Amount of Dicationic Ionic Liquid Act as a Recoverable and Reusable Organocatalyst for Asymmetric Diels-Alder Reaction This chapter deals with the development of modified MacMillan catalyst for the Diels-Alder reaction. The modified MacMillan catalyst was synthesized in two steps from (L)-phenylalanine as a starting material. The modified MacMillan catalysts were characterized by ^{1}H-NMR, ^{13}C-NMR, HRMS, and IR spectroscopy. We have also synthesized the dicationic ionic liquids using 1,5-dibromopentane and N-methyl imidazole. The synthesized imidazolidin-4-one, a modified MacMillan catalyst with a catalytic amount of dicationic ionic liquid were evaluated in the asymmetrie Diels-Alder reaction. The Diels-Alder reaction between cyclopentadiene and α, β-unsaturated aldehydes gave cycloaddition products in 69-96% yields with up to 90% ee of *exo* products. The catalyst was successfully recovered and reused up to 5 cycles with slightly drop in conversions as well .Chapter 3: DABCO-based Chiral Ionic Liquids as Recoverable and Reusable Organocatalysts for Asymmetric Diels-Alder Reaction Chapter 3 deals with the synthesis and characterization of DABCO-based novel chiral ionic liquids, and their application in asymmetric Diels-Alder reaction. The DABCO- based chiral ionic liquids were characterized by NMR, HRMS, FT-IR, and TGA. These chiral ionic liquids were evaluated as organocatalysts (5 mol%) for the asymmetric Diels-Alder reaction between crotonaldehyde and cyclopentadiene at 25 °C and the hydrophobic chiral ionic liquid containing hexafluorophosphate anion afforded product in exo/*endo* (1/1.2) in 98%

conversion with 87% ee (endo). The catalyst was recovered and reused up to 6 cycles with a slight drop in conversion and *ee* of the product due to the physical loss of the catalyst. Chapter 4: Enantioselective Friedel-Crafts Alkylation of Indoles with af-Unsaturated Aldehydes Catalyzed by Recyclable Second generation MacMillan Catalyst Chapter 4 deals with the synthesis and characterization of novel imidazolium ionic liquids derived from the second-generation MacMillan catalyst, and their application in the enantioselective Friedel-Crafts reaction of N-substituted indoles with αβ-unsaturated aldehydes. The synthesized chiral ionic liquids were characterized by various techniques such as NMR, FT-IR, TGA, and HRMS. The chiral ionic liquid containing hydrophilic bromide anion (10 mol%), co-catalyst trifluoroacetic acid (10) mol%) gave 3-alkylated *N*-protected indoles in 43-95% yields with 58-90% enantiomeric excesses. The chiral ionic liquid was recovered and reused up to 4 recycles but the significant loss in yield and ee was observed after the 3rd recycling due to degradation of the catalyst. Chapter 5: Imidazolium Ionic Liquid containing First Generation MacMillan Catalyst as a Recoverable and Reusable Organocatalyst for Enantioselective Friedel-Crafts Alkylation of N-Pyrroles with αβ-Unsaturated Aldehydes . This chapter deals with the synthesis of (S)-1-methyl-3-(5-oxo-5-((4-((1,2,2-trimethyl-5-imidazolidin-4-yl)methyl)phenyl)amino) pentyl)-1H-imidazol-3-ium ions and (S)-1-methyl-1-3-(5-oxo-5-(4-((1,2,2-trimethyl-5-oxoimidazolidin-4-yl)methyl)phenoxy)pentyl)-IH-midazol-3-ium ions. The chiral ionic liquids were characterized by FT-NMR, HRMS, and FT-IR techniques. These chiral ionic liquids were used for the first time in the enantioselective Friedel-Crafts reaction of N-methyl pyrroles and α, β-unsaturated aldehydes. The modified chiral ionic liquids were evaluated in the asymmetric Friedel-Crafts reaction using TFA as a co-catalyst in THF:H2O (95:5) at -30 °C. The chiral ionic cliquid (10 mol%), TFA (10 mol%) gave 2-alkylated N-protected pyrroles in 53-78% yields with 63-83% enantiomeric excesses. The chiral ionic liquid was recovered and reused up to three cycles.

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1. Genreal introduction to chirality and asymmetric Diels-Alder and Friedel-Crafts reactions 2. Chiral imidazolidin-4-one with catalytic amount of dicationic ionic liquid act as a recoverable and reusable organocatalyst for asymmetric Diels-Alder reaction 3. DABCO-based chiral Ionic liquids as recoverable and reusable organocatalysts for asymmetric Diels-Alds reaction 4. Enantioselective friedel-crafts alkylation of indoles with α,β-unsaturated aldehydes catalysed by recyclable second generation MacMillan catalyst 5. Imidazlium ionic liquid containing first generation Macmillan catalyst as a recoverable and reusable organocatalyst for enantioselective friedel-crafts alkylation of N-Pyrroles α, β-unsaturated aldehydes.

02. ANKIT KUMAR
Novel Approaches for the Synthesis of 4–Aminoquinolines, 1-H-Pyrroles, Maleimide Derivatives via Ynones and Hydrothiolation of gem-Difluoroalken.
Supervisor: Prof. Akhilesh K. Verma
Th 26580

Abstract

We have demonstrated an efficient base–promoted annulation of ynones with 2–amino benzonitrile to prepare multisubstituted 4–aminoquinolines and 4–amino–1,8–naphthyridines in good to excellent yields. The reaction proceeds via aza-Michael addition/intramolecular annulation. Additionally, N-arylquinolones were obtained when o-haloarylynones were used as substrate. Then we have described transitional-metal-, and additive/ligand-free, base–promoted synthesis of structurally diversified 2,3,4–trisubstituted pyrroles from ynones and isocyanoacetates via [3+2] cycloaddition under mild reaction conditions in good to excellent yields. Synthetically, the strategy appears to hold much promise as the developed strategy provides an atom-economical and environment–friendly route for the facile construction of a wide range of functionalized pyrroles. The developed chemistry is also successful for gram scale and functionalized bis-pyrrole derivatives. The synthetic utility of the product further extended toward the synthesis of a pyrrole-triazole hybrid molecule. We also have reported an elegant method for the N-bromosuccinimide-promoted one-pot synthesis of novel various 3-Benzoyl-4-phenyl-1H-pyrrole-2,5-dione and (2-bromo-4-phenyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone has been developed in good to excellent yields. Further, we have developed a co-catalytic method for thehydrothiolation of gem-difluoroalkene stogenerate α,α difluoro alkyl thioethers.This system substantially expand supon the existing scope of fluorine-retentive hydrothiolation of gemdifluoroalkenes ,as access to α,α-difluoroalkylthioethers derived from each distinct pairing of aliphatic and aryl gemdifluoroalkenes and thiols are enabled by this method.

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1. Base promoted synthesis of polysubstituted 4- aminoquinolines from Ynones and 2- Aminobenzonitriles under transition Metal free conditions 2. Base-Mediated Ynone-Isocyanide [3+2] Cycloaddition: A general method to 2,3,4-Tri-Substituted 1-H-Pyrroles and Bis-Pyrroles 3. NBS-Promoted detosylation, dearomatization, oxidation of 2,3,4-Trisubstituted 1H-Pyrroles: synthesis of maleimide derivative 4. A general Co-Catalytic hydrothiolation of gem-difluoroalkenes. Summary of the work. Copies of the publications.

03. ANOOP KUMAR
Fabrication of Non-Ionic Amphiphillc Nanocarriers for Biomedical Applications & Guar Gum Based Metallic Nanoparticle for Heterogeneous Catalysis.
Supervisor: Prof. Suhnil K. Sharma
Th 27071

Abstract

Title of thesis: "Fabrication of Non-ionic Amphiphilic Nanocarriers for Biomedical Applications & Guar Gum Based Metallic Nanoparticles for Heterogeneous Catalysis". The thesis is divided into four chapters, i.e. Chapter I, Chapter II, Chapter III and Chapter IV. Chapter 1: Self-assembly and transport behaviour of non-ionic fluorinated and alkylated amphiphiles for drug delivery Chapter II**:** Phloroglucinol based dendric amphiphiles: Synthesis and study of their potential as nanocarrier Chapter III**:** Synthesis of guar gum and Fe3O4 nanocomposites for photocatalytic degradation of dyes and heavy metals Chapter IV**:** Synthesis of bimetallic magnetic Pd/Cu-GGFe3O4 nanoparticles: Application in carbon-carbon cross-coupling reactions.

Contents

1. Self assembly and transport behaviour of non-ionic fluorinated and alkylated amphiphiles for drug delivery 3. Phloroglucinol based dendric amphiphiles: Synthesis and study of their potential as nanocarrier 3. Synthesis of guar gum and Fe_3O_4 nanocomposites for photocatalytic of dyes and heavy metals 4. Synthesis of bimetallic magnetic Pd/Cu@GG-Fe_3O_4 nanoparticles: application in carbon-carbon cross-coupling reaction. Summary.

04. BHAWNA
Synthesis and Applications of Engineered SnO2 Nanoparticles: Photocatalytic Water Splitting, Dye Degradation and Plastic Waste Conversion to Fuel Production.
Supervisor: Prof. Prashant Singh
Th 26581

Abstract

Global energy consumption and demands have significantly escalated over the past years. Conventional fossil fuels have led to CO2 emission, alongside other greenhouse gases and global warming. Therefore, it's the paucity to establish strategies that proves to be beneficial to meet today's energy demands and enhance development of renewal energy resources. The main objective of the current thesis is to investigate and devise new strategies for generating energy in environment friendly, and economically feasible ways. SnO2 based nanomaterials have been extensively explored in the thesis due to their higher stability and wide bandgap semiconducting properties. A complete description of its structure and properties has been elaborated for an understanding of its phase, symmetry and other characteristics. The pivotal target of the work is to investigate variation in properties of tin oxide upon cation and anion doping in terms of their photocatalytic water splitting reaction for hydrogen generation, photocatalytic dye degradation and thermocatalytic conversion of plastic waste to value added products for plastic waste management. This thesis puts forth a better research by providing a contribution of metal oxides towards environmental concerns by dealing with energy crisis and environmental pollution.

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1. Introduction 2. Effect of Ce doping on SnO2 for Hydrogen evolution through photocatalytic water splitting reaction and dye degradation 3. Novel synthesis of N doped SnO2 nanoparticles: A promising Cocatalyst free photocatalyst for hydrog 4. N, F-Codoped SnO2: An efficient photocatalyst for hydrogen generation through photocatalytic water splitting 5. Plastic waste to value added products: Low temperature mediated Thermo-Catalytic conversion using Ce doped SnO2 nanoparticles. Summary. List of Publications. List of International/National Conferences and award.

05. CHAKRABORTY (Nayanika)

Synthesis, Characterization of Photoactivated Prussian Blue- Based Nanoparticles & Their Antimicrobial Applications.

Supervisors: Prof. Indrajit Roy and Dr. Hemant Kumar Gautam

Th 26582

Abstract

The inception of antibiotics for clinical utilization has metamorphosed the face of modern medicine for treating bacterial infections. However, haphazard use, misuse and overuse of antibiotics progressively, inevitably led to rapid emergence of pathogenic strains with antimicrobial resistance (AMR). It's disgruntling to apprehend that the development of AMR has eclipsed the discovery of new antibiotics. Under these atrocious circumstances, efforts have been made to identify nanoformulations to combat AMR. Phototherapy is a lucrative recourse to ablate bacterial infections using light conditions with the benefit of dodging incidences of bacterial resistance. The research work embodied in this thesis have endorsed the utilization of Prussian blue (PB) nanoparticles (NPs), a FDA approved non toxic and exceptionally versatile nano photonic platform for the exasperating fight against the hornet's nest of bacterial infections. Foremost, we have investigated the pattern of interaction at the nano-bio interface using Chitosan-coated Prussian blue (CHPB) nanoparticles and further photo-activated them with a 635nm laser for antibacterial therapy. Further, the ability of photosensitizer (FITC-dextran) loaded chitosan coated Prussian blue nanoparticles was examined to photogenerate singlet oxygen, which is further mitigated by the catalase-like behavior of the core nanoparticles under dual and white light irradiation. These nanoparticles were also utilized for topical application on infection-mimicking cutaneous wound model. Convinced with antibacterial activity under dual and white light irradiation, we stimulated the design and development of Silver Prussian blue – Crystal violet (SPB-CV) nanocomplex, for enhanced PDT using white light photoactivation against drug resistant Gram positive strains that are prevalent cause of Hospital Acquired infections (HAIs). Lastly, in an attempt to provide an economic and innovative solution to the ever evolving outrageous problem of infectious wound healing, we impregnated Silver Prussian blue – Crystal violet nanoparticle into cotton fabrics and explored them as white light activatable bandages with superior bacterial sterilization and accelerated wound repair.

Contents

06. CHANDEL (Sakshee)
Development of Nanostructured Sodium Titanate as Promising Anode Material for Sodium Ion Battery Application.
Supervisor: Dr. Alok Kumar Rai
Th 27072

Abstract

The first chapter of current thesis entitled "Development of Nanostructured Sodium Titanate as Promising Anode Material for Sodium Ion Battery Application" highlights the requirement of batteries along with their backgrounds. Thereafter, we have discussed sodium ion batteries (SIBS) followed by its working mechanism and the challenges. Then, the various types of SIB anode materials along with their merits and demerits are summarized. At last, we have covered the unique features of sodium titanate as an anode material for SIB applications. The second chapter of the thesis focuses on the various synthesis methods such as solvothermal, sol-gel, polyol-assisted pyro synthesis method, which are used for fabrication of sodium titanate anode materials. The electrode fabrication of synthesized active materials followed by coin cell assemblies are also discussed. Further, this chapter provides a brief overview of the characterisation techniques that are used to systematically analyse the fabricated electrode materials. Third chapter describes the synthesis of a unique two phase $Na_2\ Ti_6O_{13}/Na_2Ti_3O_7$ nanocomposite using facile solvothermal method and then the synthesized nanocomposite is tested as an anode material for SIB application. The superior electrochemical performances of two phase $Na_2\ Ti_6O_{13}/Na_2Ti_3O_7$ nanocomposite than the single phases can be ascribed to the synergetic effect between $Na_2Ti_{16}O_{13}$ and $Na_2Ti_3O_7$, phases that could effectively nullify the drawbacks of individual phases and thereby these phases act as complement to each other. The impact of optimized Mo doping on sodium titanate anode is further revealed in the fourth chapter of the thesis. In order to find a suitable electrolyte system for Mo-doped sodium titanate electrode, the various electrolytes were tested. Among all the electrolyte systems, the most compatible electrolyte was found to be $NaPF_6$, in diglyme. The incorporation of Mo^{6+} into the crystal structure of sodium titanate leads to the partial reduction of Ti^{4+} to Ti^{3+} along with the creation of oxygen vacancies. The combined effect of both the extra electron of Ti^{3+} and oxygen vacancies significantly improves the electrical conductivity as well as Na^+ ion storage kinetics, resulting the excellent electrochemical performances of Mo doped sodium titanate anode for SIBS. The fifth chapter describes a doping of vanadium (V^{5+}) in sodium titanate nanorods synthesized by sol gel method. It was clearly observed that V^{5+} doping significantly affects the phase formation of sodium titanate samples, which leads in alteration of the major phase of $Na_2Ti_3O_7$, to single phase of $Na_2Ti_6O_{13}$ with increase of doping concentrations. Similarly, like Mo doping, the incorporation of highly charged V^{5+} ions in sodium titanate lattice produces oxygen vacancies along with the partial reduction of Ti^{4+} to Ti^{3+}, resulting the improved electronic conductivity. It is also believed that the utilization of oxygen vacancies preserves the integrity of the electrode and helps to achieve long range cycling. The sixth chapter summarized the synthesis of sodium titanate/reduced graphene. oxide (rGO) nanocomposite via a two-step solvothermal method. Pure sodium titanate was also synthesized for comparative studies. The morphological analysis revealed that the rGO nanosheets are well imbedded with the hierarchically arranged nanorods of

$Na_2Ti_6O_{13}$. The nanocomposite exhibits better electrochemical properties than the pure sodium titanate due to the tight integration between rGO and $Na_2Ti_6O_{13}$. The rGO nanosheets offer the electrically conductive paths for fast movement of Na^+ ions and also act as buffer to accommodate the volume variations during (de) sodiation. In the seventh chapter, a rare phase of $Na_{0.23}TiO_2$ nanoparticles wrapped within full carbon network was successfully synthesized via a highly efficient polyol assisted pyro synthesis method. The polyol used in the synthesis method acts not only as a solvent, low-cost fuel, reducing agent but also acts as a carbon source to form the carbon network. Morphological analysis clearly displayed that $Na_{0.23}TiO_2$ nanoparticles are fully covered within the carbon network. The obtained $Na_{0.23}TiO_2/C$ exhibits excellent rate capability and long cycling stability as an anode for SIB application due to the carbon network that provides the conductive medium to reduce the path lengths of ions/electrons.

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1. Introduction 2. Synthesis procedures and experiemental details 3. Fabrication of hybrid nanocomposite of sodium titanate as an anode for superior electrochemical performances 4. High reversible capacity induced by M0-doping in sodium titanate anode for rechargeable sodium ion battery application 5. Effect of vanadium doping on electrochemical performances of sodium titanate anode for sodium ion battery application 6. Reduced grapheme oxide (rGO) integrated sodium titanate nanocomposite as high rate performance anode for sodium ion batteries 7. One-step synthesis of a rare polymorph of sodium titanate ($Na_{0.23}TiO_2$) anode wrapped within full carbon network. Summary. Futurue scope. List of publications.

07. CHATURVEDI (Chhaya)
Development of Electrochemical Biosensors for Neurotransmitter-Serotonin Detection. Acute and Post Acute Covid-19 Manifestations.
Supervisor: Prof. Ramesh Chandra
Th 27073

Abstract

During last five decades, Biosensor become quite popular due to their important role in the sensitive, selective, quick and cost-effective detection of various diseases. Since then, continuous efforts are being made by various reaserch groups to develop an efficient electrochemical biosensing point of care chip for specific disease detection. For this, tuning with either transducing material such as one-dimensional (ID), two- dimentional (2D), three-dimensional (3D) biorecognition or (monoclonal/polyclonal antibodies, enzymes, single stranded DNA, single stranded RNA, aptamers etc) have been used. To monitor mental health status of an individual. efforts have been made to detect serotonin concentration in biological fluids (urine. whole blood, sweat, CSF). In recent research, it has been reported that COVID-19 pandemic directly or indirectly impact mental health status of the individuals. According to the WHO, one billion people suffer from mental disorders, over 280 million individuals experience depression, regardless of age, and one person commits suicide every second. Furthermore, scientific data is emerging on the potential impact of COVID-19 on people with mental issues, as well as the psychological impact on isolated people and healthcare staff. Medical study shows that COVID-19 patients may have

both short-term and long-term mental health problems. Cognitive, vertigo, depression, anxiety, altered awareness, agitation, traumatic stress, and insomnia have been described in COVID-19 patients. Alterations in neurotransmitters such as melatonin, dopamine, histamine, serotonin, and others are usually associated with these problems. Serotonin, along with norepinephrine and GABA, is one of the three major neurotransmitters associated with anxiety. Potentially traumatic patients have consistently low serotonin levels, which lead to lethargy, feelings of hopelessness, poor memory, neurological disorder, restlessness, and psychotic symptoms. Changes in serotonin concentrations in bodily fluids might possibly play a role in COVID-19 pathophysiology. This research work was mainly focused on fabricating, designing and modifying graphitic carbon nitride (g-CsNa) for an efficient photocatalytic degradation of various notorious pollutants. The idea of current research work was to investigate the capability of the graphitic carbon nitride, graphitic carbon nitride-based nanocomposites as a photocatalyst and catalyst, for the eradication of rhodamine B (RhB) dye, Nitro compound and tetracycline (TC) antibiotic pollutant.

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1. Introduction 2. Review of literature 3. Aims and objective 4. Nanostructured molybdenum selenide-reduced grapheme oxide based biosensor for serotonin detection 5. Nanostructured molybdenum disulphide-reduced grapheme oxide based biosensor for serotonin detection 6. Nanostructured molybdenum ditelluride-reduced grapheme oxide based biosensor for serotonin detection 7. Doped nanocomposite based point of care device for serotonin detection. Summary.

08. CHAUDHARY (Pooja)
Development of Recoverable Chiral Mn(III)-Salen Complexes For Enantioselective Organic Transformations and Enantiomeric Excess Determination of Amines.
Supervisor: Prof. Surendra Singh
Th 27074

Abstract

The thesis reveals the synthesis of new homogeneous chiral Mn(III)- salen complexes, ionic liquid tagged chiral Mn(III)-salen complexes, heterogeneous chiral Mn(III)-salen COF, and enantiopure BINOL-derived chiral solvating agents (CSAs). The chiral homogeneous and heterogeneous Mn(III)-salen complexes were applied in different asymmetric organic transformations such as enantioselective epoxidation of olefins and oxidative kinetic resolution of racemic secondary alcohols.. The enantiopure BINOL-derived CSAS were used for the enantiopurity determination of primary and secondary amines via 'H- and "F-NMR spectroscopic analysis. Chapter 1 covers the general introduction of chirality and different methods to synthesize the optically active compounds. Chapter 2 consists of the synthesis and characterization of homogeneous chiral Mn(III)-salen complexes and their application in the asymmetric epoxidation of styrenes and chromenes. The complexes derived from (1R,2R)-1,2-diphenylethylenediamine found to be more reactive and enantioselective compared to the complexes, which were synthesized from (1R,2R)-1,2-diaminocyclohexane. The asymmetric epoxidation of styrenes and

chromenes in ethyl acetate using these Mn(III)- salen complexes as catalysts in the presence of pyridine-N-oxide, afforded the corresponding epoxides in 95-98% yields with 29-88% ee's at 0 °C. The catalysts were easily recovered and reused in the asymmetric epoxidation of styrene with the gradual decrease in the yield of styrene oxide and ee remain consistent in each run.Chapter 3 described the synthesis and characterization of chiral ionic liquid (IL) tagged Mn(III)-salen complexes and their application in the oxidative kinetic resolution (OKR) of various racemic secondary alcohols. The chiral complexes, containing hydrophobic [PF anion shows good enantioselectivity as compared to the complexes, having hydrophilic [Br] and [BF] anions. The OKR of ortho-, meta-, and para-substituted benzylic alcohols were carried out and the corresponding resolved products were obtained with up to 99% ee. Catalyst was easily recovered and reused for 5 times in the OKR of (+)-1-phenylethanol without significant loss of activity and enantioselectivity. Chapter 4 covers the synthesis and characterization of 3,3'-disubstituted (S)-BINOLS from (S)-BINOL and their utilization as chiral solvating agents (CSAS) to determine the enantiopurity of primary and secondary amines via ^{1}H- and ^{19}F-NMR spectroscopic analysis. The synthesized (S)-BINOL derivatives were evaluated as CSAs to determine the enantiodifferentiation of various types of amines. In this protocol, the analyte and CSA were directly mixed in an NMR tube in chloroform-d and after shaking for 30 seconds the ^{1}H- and ^{19}F-NMR spectra were recorded, which affords well-resolved resonance peaks for both the enantiomers present in an analyte. The enantiomeric excess of 1,2-diphenylethylenediamine was determined and a linear relationship with the coefficient of R^2 = 0.9995 was observed. This protocol is very efficient and less time-consuming as compared to the derivatization protocol. Chapter 5 described the synthesis of two-dimensional chiral salen-based covalent organic framework (COF) via rapid microwave-promoted condensation of C3-symmetric 1,3,5-tris[(5-tert-butyl-3-formyl-4-hydroxyphenyl)ethynyl]benzene with (1R,2R)-1,2-diaminocyclohexane and $Zn(OAc)_2.2H_2O$ in less time and slightly high yield (77%) at 120 °C. The synthesized chiral salen-COF showed 454 m^2g^1 BET surface area with excellent crystallinity and thermal stability. Further, the post-synthetic metal exchange reaction of chiral salen-COF with $Mn(OAc)_2.4H_2O$ provided the chiral Mn(III)-salen COF in good yield (89%) and it was utilized as an effective heterogeneous catalyst for the asymmetric epoxidation of unfunctionalized olefins. The synthesized chiral Mn(III)-salen COF (5 mol%) catalyzed the enantioselective epoxidation of unfunctionalized olefins and afforded the corresponding epoxides in 87-98% yields with 10-72% ee's. The chiral Mn(III)-salen COF easily recovered by centrifugation and reused up to four cycles in the enantioselective epoxidation of 2,2- dimethyl-2H-chromene with a loss of activity but enantioselectivity remains consistent in each catalytic cycle.

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1. Introduction 2. Synthesis of new chiral Mn(III) salen complexes as recoverable and reusable homogenous catalysts for asymmetric epoxidation of styrenes and chromenes 3. Synthesis of chiral Mn(III) salen complex tagged with ionic liquid as recoverable and reusable homogenous catalysts for oxidative kinetic resolution of secondary alcohols 4. A simple protocol for determination of enantiopurity of amines using BINOL derivatives as chiral sovating agents via ^{1} H- and ^{19} F-NMR spectroscopic analysis 5. Synthesis and characterization of chiral salen covalent organic framework and its

Mn(III)-salen complex as heterogenous catalyst for enantioselective epoxidation of styrenes and chromenes. Summary. List of publications.

09. CHAUHAN (Dipti)
Development Of Nanomaterials Based Biosensors For Liver Cancer Detection.
Supervisor: Dr. Suveen Kumar
Th 27075

Abstract

Nanomaterials owing to their exciting properties such as high surface area, excellent electronic conductivity, ease of functionality, ultralight weight, high mechanical strength, etc. have gained immense attention among researchers to utilize them in a wide variety of applications including biosensors. They are efficiently employed as immobilization matrix in the fabrication of biosensors for various diseases detection. Among different kinds of nanomaterials, carbonaceous nanostructures such as graphene, graphene oxide, carbon nanotubes, porous carbon etc. have anticipated researchers across the globe for development of biocompatible, cost effective and metal free non-toxic biosensing platforms. Among these, multi-walled carbon nanotubes (MWCNTs) have played an immense role as excellent electrode materials to improve the performance of electrochemical assay. These are rolled layers of few grapheme sheets with diameter upto 100 nm. They possess excellent electronic conductivity, high charge transfer capability, large surface area, wide electrochemical potential window, good biocompatibility and high mechanical stability. Along with these carbonaceous materials, recently, an interlinked organic framework enriched with □-electrons i.e., hydrogen substituted graphdiyne (HsGDY), is introduced as a rising star with high conjugation, comprising of repeating structural units of a big hexagonal ring assembled by 42 carbon atoms, each unit composed of six benzene rings (sp2 hybridized) interlinked by diacetylenic linkages (-C□C-C□C-; sp hybridized), thereby furnishing it with uniform in-plane cavities distributed throughout the structure. This synthetic carbon allotrope differs in structure and properties from other carbon allotropes due to presence of sp as well as sp2 hybridized carbon atoms which leads to inhomogeneous -bondings, thus ensuing natural band gap in semiconducting range. Additionally, it is endowed with high intrinsic carrier mobility (upto 105 cm2 V-1 s-1) due to the presence of dirac points and cones; thus suggesting high conductivity reaching upto 103 S m-1. The presence of sp hybridized carbon atoms results in more favourable and stronger interaction of biomolecules with GDY and its counterparts as compared to graphene.Furthermore, the hierarchical pores provide additional pathway for facile diffusion of ions perpendicular to the molecular plane; unlike the steric hindrance caused in graphene due to sp2 hybridized carbons. Thus, these sp-circumferenced cavities provide 2 tunnels for electrons hopping, high surface area and strong adsorption ability for loading of biomolecules, that helps in amplifying the signal to noise ratio of electrochemical signals and lead to enhanced sensitivity and quick response. Keeping these properties in view, we have used two nanomaterials, i.e., MWCNTs and HsGDY in our research work for the development of biosensors for liver cancer detection. Cancer characterized by aberrant cell growth in an unregulated manner, is the leading cause of death worldwide with third position occupied by liver cancer (LC),reporting 8,30,000 deaths in 2020. The LC is associated with risk factors like cirrhosis,chronic viral hepatitis B and C,

non-alcoholic fatty liver disease and consumption of food toxins such as aflatoxin. Presently, the techniques used for surveillance are examining blood α-feto protein (AFP) levels with a follow-up diagnosis using imaging scans (ultrasonography, CT-scan, hepatic angiography, laparoscopy) and biopsy.However, these imaging techniques are challenged by less sensitivity, radiation hazards, expensive instrumentation, contrast injury, visualization of large sized nodules (>3 cm) and appearance of disguised nodules mimicking LC in cirrhotic patients, that limits their use for precise diagnosis. On the other hand, biopsy remains a highly invasive tool for detection of cancerous lesions. In this context, electrochemical biosensors emerge as a rapid, highly sensitive, cost-effective and easy miniaturized platform to detect LC at one's fingertips.

Contents

1. Introduction 2. Experimental details and instrumentation 3. Amine functionalized multi-walled carbon nanotubes based biosensor for liver cancer detection 4. Hydrogen substituted graphdiyne based bionsensor for liver cancer detection 5. Amine functionalized substituted graphdiyne based biosensor for liver cancer detection 6. Hyudrogen substituted graphdiyne oxide based biosensor for liver cancer detection. Summary and future prospects. Refernces.

10. CHOUDHARY (Renu)
Synthesis of Pyridines and Benzo-Fused Pyridines Through Oxidative Condensation and Coupling Methodologies.
Supervisor: Dr. K. Gopalaiah
Th 26583

Abstract

The thesis consists of five chapters, and deals with the research work related to oxidative condensation and annulation of various amine and hydrocarbon nucleophiles in the presence of sustainable metal catalysts or metal-free catalytic reaction conditions to produce 2,4,6-triaryl pyridines, 4-aminoquinolines and 9-aminoacridines. Chapter I illustrates a brief literature review on the recent developments related to the construction of aromatic six membered N-heterocyclic compounds especially pyridines and benzo-fused pyridines. Various synthetic methodologies for the preparation of pyridine derivatives such as quinolines, isoquinolines, acridines and phenanthridines are presented. Furthermore, this chapter highlights the importance of these heterocycles in various fields such as pharmaceuticals and material science. The synthetic methods are divided into two categories on the basis of catalytic system (i) metal-catalyzed and (ii) metal-free synthetic methods which mainly proceed through oxidative condensation, cross-coupling and annulation reactions. Chapter II deals with the iron-catalyzed acrobic oxidative cascade annulation of arylacetylenes with benzylamines for the synthesis of 2,4,6-triaryl pyridines. The reaction was performed using iron(II) triflate as a catalyst and molecular oxygen as a green oxidant under solvent-free conditions. Scope of the reaction was studied thoroughly by employing several electron-donating and electron-withdrawing groups on the aryl ring of phenylacetylenes and benzylamines to afford the functionalized unsymmetrical and symmetrical 2,4,6-triaryl pyridines in good to excellent yields. In this reaction, benzylamine acts as a

sole nitrogen source for the construction of Krohnke pyridines. Some control experiments were conducted to understand the mechanism of the oxidative reaction. The proposed mechanism involves the generation of propargylamine intermediate, capturing of ammonia, and 6-endo-dig cyclization to form the desire product. Chapter III demonstrates a tandem oxidative coupling and annulation approach for the construction of novel *N*-benzyl-2-phenyl-4-quinolinamines using o- aminoacetophenones and benzylamines in one-pot method. The reaction was proceeded in the presence of FeBr2 catalyst under molecular oxygen atmosphere in xylene at 120 °C. The generality and substrate scope of the reaction was investigated with various o-aminoacetophenones and benzylamines to obtain the corresponding quinoline products in good to excellent yields. Several control experiments were performed to isolate the intermediates such as N-benzyl-1-phenylmethanimine, (E)-1- (2-aminophenyl)-3-phenyl-2-propen-1-one and 2-phenyl-2,3-dihydroquinolin-4(1H)- one. Mechanistic investigations revealed that the present protocol is based on the oxidative condensation of benzylamine to form N-benzyl-1-phenylmethanimine, Claisen-Schmidt type condensation reaction with o-aminoacetophenone followed by cyclization to form 2-phenyl-2,3-dihydroquinolin-4(1H)-one. This intermediate undergoes oxidative condensation with another molecule of benzylamine to furnish the desired product. It is worthy to mention that the compounds prepared by this methodology are novel and structure of these products were confirmed by single crystal X-ray diffraction analysis, NMR and HRMS data. The synthetic utility of the present method was demonstrated by preparing N-(4-chlorophenyl)-2-phenylquinolin- 4-amine and N^1,N^1-Dimethyl-N^2-(2-(4-methylphenyl) quinolin-4-yl)ethane-1,2- diamine (graveoline derivative) possessing antifungal and anticancer properties, respectively. Chapter IV deals with the metal-free oxidative annulation for the synthesis of N-benzyl-2-phenyl-4-quinolinamine scaffolds using o-aminoacetophenones and benzylamines in one-pot procedure. Reactions were conducted with stochiometric amount of DMAP (4-(N,N-dimethylamino)pyridine) and TBHP (tert-butyl hydroperoxide) at 100 °C under neat conditions for successful oxidative condensation of benzylamines with o-aminoacetophenones to obtain the functionalized 4- aminoquinolines in good to high yields. The structure of the products was analyzed by single crystal X-ray studies, ^{1}H and ^{13}C NMR and HRMS spectral data. Furthermore, some control experiments were conducted to gain insight into the reaction mechanism and plausible mechanistic pathway has been designed based on the isolation of the homo-imine and 2,3-dihydroquinolone key intermediates. Chapter V describes the construction of 9-aminoacridine framework through one-pot sequential Buchwald-Hartwig coupling followed by Lewis-acid mediated cycloaromatization by using commercially available 2-bromobenzonitriles and anilines as starting materials. The Buchwald-Hartwig amination was conducted with $Pd(OAc)_2$ catalyst, rac-BINAP ligand and Cs_2CO_3 base in xylene at 100 °C, and cycloaromatization was proceeded with boron trifluoride etherate ($BF_3.OEt_2$) in xylene solvent at 100 °C to furnish the 9-aminoacridine compounds. A variety of substituted 2-bromobenzonitriles were well tolerated under the optimized reaction conditions to furnish the corresponding products in moderate to good yields. Subsequently, various anilines bearing electron donating as well as electron withdrawing groups on the aryl ring were employed for this transformation to afford the desired products in 72-94% yields. Additionally, we have isolated the Buchwald- Hartwig amination intermediate and proposed the reaction mechanism.

Contents

11. CHUGH (Heerak)

Microtubule Targeting Agent: Noscapine - A Dynamic Cancer Therapeutic.

Supervisors: Prof. Satish Kumar Awasthi, Prof. Ramesh Chandra and Dr. Rajesh K. Gaur

Th 26584

Abstract

Cancer is a disease that is characterized by masses of unregulated growth called tumours with the ability to metastasize. It's no surprise to the current population as to why the incidences of cancer rates have increased globally. The mortality rates have declined to a mild extent as we progress with cancer research and pharmaceutical development. However, these approaches need to be more advanced as either they are very toxic to the non-tumorous cells and do more harm than good or cancer cells are developing resistant against these drugs rendering them useless. Thus, there have been increasing needs for better chemotherapeutic drugs- that are less toxic but are as effective at curbing the anti-proliferative potential of the tumour in question. Among the many chemotherapeutic agents available with better anti-cancer potential, Noscapine stands out with its minimal toxicity to major organs of the body and low immunogenic ability. All these factors added to the existing advantages with pursuing Noscapine as a potential anti-cancer agent- it is effective in resistant tumours where the conventional drugs have failed, multiple intervention points in cancer physiology and, is applicable and effective in wide range of cancers. A drawback with Noscapine is its short half-life and thus reduced bioavailability in blood plasma. In my thesis I have hypothesized and evaluated formulations of Noscapine that may increase its pharmacological relevance as an anti-cancer agent and evaluated the non-specific interactions which may affect Noscapine's ADMET profile – these have helped us to specifically modulate the chemical structure of Noscapine to optimize non-specific binding but maintaining blood plasma levels. We were also able to establish potential novel anti-cancer agent as inhibitors of HYPE through international collaborations. In conclusion, we were able to move a step forward to establish potential anti-cancer chemotherapies and finding answer to a global problem- Cancer.

Contents

fluorouracil in *in vitro* models of non-small cell lung cancer 5. Synthesis, characterization and evaluation of anti-cancer efficacy of multicomponent noscapine loaded collagen stabilized silver nanoparticles 6. Interaction of noscapine with human serum albumin (HSA): a spectroscopic and molecular modelling approach 7. Ex vivo binding studies of the anti-cancer drug noscapine with human hemoglobin: A spectroscopic and molecular docking study 8. Small molecule manipulators of hype-mediated ampylation: validation of novel cancer therapeutics 9. Summary.

12. DEEPAK KUMAR

Exploration of Novel Polyxometalate Based Hybrid Materials for Supercapacitive Charge Storage.

Supervisor: Prof. RajKishore Sharma

Th 27076

Abstract

In today's world, we rely primarily on electricity for the majority of our everyday needs, including everything from technological devices to transportation infrastructure. As a result of global concerns over existing energy policy, a paradigm shift from non-renewable to renewable energy resources policy is necessary. The most demanded solutions for real-world electronic devices are batteries and supercapacitors. Supercapacitors have high-power density with low energy density whereas batteries have a high-power density with low energy density. Based on the charge storage mechanisms supercapacitors are classified as electric double layer capacitors (EDLCs) and pseudocapacitors (PCs). Nowadys, a new class of redox active materials capable of multielectron transfer without any structural change, called polyoxometalate (POM) is emerging. In the entire work, our focus was on designing novel out of the box pathways for the less explored POMs to showcase their tremendous potential to meet real world energy requirements. In Chapter 1, we have discussed supercapacitors and their importance along with charge storage mechanisms and different types of materials that can be used. This chapter also covers introduction to POMs and how they are prominent candidates for charge storage, followed by various methods for synthesis. Chapter 2, covers various characterization techniques (structural, morphological and electrochemical) used for polyoxometalate based hybrid materials. In chapter 3, we have reported a strategy to extend the operating potential by utilizing ammonium decavanadate-holey reduced graphene oxide nanoribbons (rGONR-ADV) as hybrid electrode for supercapacitors. In chapter 4, we incorporated ADV to investigate the effect of interlayer distance on the electrochemical performance of α-Co(OH)2 nanoplates (ACH). Chapter 5 highlights application of POMs for designing advanced materials with need tailored morphology. A precise control over morphology and properties always remained a challenging task. In chapter 6, instead of directly using POM, we utilized a bimetallic substituted POM to derive metal sulfide nanosheets.

Contents

1. Introduction 2. Characterization techniques 3.Ammonium decavanadate nanodots/reduced grapheme oxide nanoribbon as "inorganic-organic" hybrid electrode for high potential aqueous symmetric supercapacitors 4. Interlayer gap widened 2D α-$Co(OH)_2$ nanoplates with decavanadate anion

for high potential aqueous supercapacitors 5. Polyoxometalate/ZIF-67 composite with exposed active sites as aqueous supercapacitors electrode 6. Polyoxometalate derived TMDs deposited MXene nanosheets as high-performance aqueous supercapacitors 7. Conclusion. List of publications.

13. DEY (Priya)
Dynamics and Aggregation Propensity of Intrinsically Disordered Proteins.
Supervisor: Prof. Parbati Biswas
Th 27209

Abstract

A large number of proteins in eukaryotes belong to intrinsically disordered proteins (IDPs). Such proteins typically exist as a dynamic ensemble of interconvertible conformations under physiological conditions and are implicated in a wide variety of cellular processes. These proteins are involved in many diseases that include neurodegenerative disorders and some forms of cancer. Elucidating the molecular mechanisms and driving forces involved in protein aggregation has therefore been a central issue for understanding and preventing protein aggregation diseases. In this thesis, different techniques are used to study the aggregation propensity, relaxation dynamics, and the mechanism of protein aggregation and its inhibition. The effect of intrinsic disorder on the hydration thermodynamics and aggregation propensity of proteins is studied using MD simulations and 3D-RISM theory. The aggregation propensity is also measured using the global and local relaxation dynamics of the disordered protein amyloid-β and its naturally occurring mutants. Its aggregation is explored using a statistical potential through the Monte Carlo simulations. The aggregation of amyloid-β causes Alzheimer`s disease which is a detrimental neurological disorder characterized by the formation of amyloid fibrils due to the aggregation of amyloid-β. Primary therapeutic approaches for treating Alzheimer`s disease are targeted to prevent this amyloid fibril formation using potential inhibitor molecules. Therefore, the effect of a naturally occurring inhibitor, caffeine, on the dimer of the full-length amyloid-β is investigated in this thesis. Our results provide new insights for understanding and predicting the protein aggregation propensity, thereby offering novel design principles for producing aggregation-resistant proteins for biotherapeutics.

Contents

1. Introduction to electrode surface 2. Aggregation Propensities of Proteins with Varying Degrees of Disorder 3. Relaxation Dynamics Measure the Aggregation Propensity of Amyloidβ and its Mutant 4. Exploring the Aggregation of Amyloid-β 42 through Monte Carlo Simulations 5. Effect of Caffeine on the Aggregation of Amyloid-β - A 3D RISM Study. Bibliogrpahy.

14. GOEL (Himanshi)
In Situ Electrochemical Determination of Morphological Characteristics of Electrode: RMS Roughness, Roughness Factor, Surface Convexity and Atomic Step Density.
Supervisor: Prof. Rama Kant
Th 26585

Abstract

In electrochemistry the electrode surface plays an important role in govering the electrochemical response. The electrode surface gets inherited roughness in the cleaning process and sometimes the roughness is also desired to alter the electrochemical properties. Thus to explain quantitatively the electrochemical response this electrode roughness needs to be characterized. This chapter review the following topics (1) different methods of roughening of metal elerctrodes, (ii) quantitative methods for roughness characterization (iii) surface characterization techniques (iv) Fundamentals of electrochemical techniques,cyclic voltammetry (CV) and (V) factors influencing electrochemical response, viz solution resistance,applied potential, electrolyte's ion size solution viscosity and temperature.

Contents

1. Introduction to electrode surface characterization using Ex-situ and In-Situ method 2. Electrochemical impendence spectroscopic method for In-Situ determination of RMS roughness 3. Chronoamperometric method for In-Situ determination of RMS roughness 4. Electrochemical impedance spectroscopic method for In-situ determination of roughness factor and morphological convexity at OHP 5. Experimental corroboration of EDL theory with varying Ion size, viscosity and temperature ar rough and porpous electrode 6. Modular theory for EIS of electron transfer with electric double layer 7. Experimental investigation of PZC for nanoparticle deposited rough electrode 8. Summary and future perspective.

15. GOYAL (Hina)
Polycyclic Aromatic Hydrocarbon-Based Soft Materials: Gel, AIEE, Mechanochromism and Sensing Properties/Applications.
Supervisor: Prof. Rajeev Gupta
Th 27077

Abstract

Polycyclic Aromatic Hydrocarbons (PAHs) and their derivatives offer notable properties which make them significant for various applications. The n-electron delocalization in PAHs enables self-assembly via - stacking which further endows PAH-derivatives with the important characteristics of soft materials while supporting gelation, aggregation-induced enhanced emission (AIEE), and mechanochromism. In addition, PAHs are widely used as fluorophore(s) due to their high emissivity which has been utilized for the detection of various analytes including metal ions, anions, neutral molecules, antibiotics, amino acids, and even explosives. Therefore, PAH-based compounds not only offer noteworthy structural properties but also remarkable applications. The aim of the present dissertation is to explore and showcase the significance of various PAH-based soft materials. In particular, the influence of assorted PAH- derivatives on gelation, AIEE, and mechanochromism has been discussed. Additionally, such soft materials were also utilized for the detection of various analytes. This dissertation has been divided into six chapters. Chapter 1 is introductory in nature and discusses selected examples of PAII containing compounds based on naphthalene, anthracene, pyrene, and naphthalene-diimide and their utilization in gel formation, AIEE, mechanochromism, and fluorescence sensing. Chapter 2 discusses the stepwise design and synthesis of a set of closely related amide-based compounds, L1-L3, which can potentially act as low-molecular-weight gelators (LMWGs). L3 was found to form a stable gel that was characterized using an array of spectroscopic, rheological and imaging techniques. Moreover, L3 not only illustrated the nanomolar sensing of a few antibiotics but also formed a much more stable gel in the presence of such antibiotics. Chapter 3 presents the same set of amide-based compounds, L1-L3, decorated with H-bonding functional groups and pyrene rings making them electron-rich in nature. All three compounds were utilized for the sensitive and selective sensing of electron-deficient picric acid (PA). LMWG L3 formed a more stable and stronger gel in the presence of PA. Chapter 4 discusses a systematic study of three closely related Schiff bases L4-L6 for their potential AIEE, gelation and mechanochromic properties. Out of three compounds, L5 and **L6** displayed AIEE due to the suppression of photoinduced electron transfer (PET). Notably, only L6 was able to form a stable gel and exhibited reversible mechanochromism. To understand the mechanism behind mechanochromism, three control molecules, L7-19, were synthesized which were structurally similar to L6 but lacked some of the H-bonding groups and did not display mechanochromism, L6 was further utilized to illustrate noteworthy anti-counterfeiting and pressure-induced applications. Chapter **5** presents two Schiff base-based chemosensors, L10 and L11. decorated with electron-rich quinoline and anthracene rings. Chemosensor L10 displayed AIEE and exhibited sensitive, selective and reversible 'turn-on' detection of Al and Gations as well as aspartic acid (Asp). Chemosensor L11, an isomer of L10, was able to selectively detect Ga^{3+} ion even in the presence of Al^{3+} ion and thus was able to discriminate between the two ions. The 'turn-on' nature of fluorescence sensing by the two chemosensors enabled the development of colorimetric, filter- paper-based test-strip and polystyrene film-based detection techniques. Chapter 6 presents a multi-arene-based electron-rich chemosensor L12 which was utilized for the sensitive and selective detection of PA over other nitroaromatic compounds (NACs). The 'turn-on' emission sensing of PA took place via chemodosimetry which was confirmed by a series of spectroscopic and life-time studies. Chemosensor L12 was further utilized for the detection of PA in the solid state.

Contents

Introduction: selected examples of polycyclic aromatic hydrocarbon based soft materials and their properties/Applications 2. Systematic design of a low-molecular-weight gelator and its applications in the sensing and retention of residual antibiotics 3. Sensing and formation of a stable Gel in the presence of picric acid by a low-molecular weight-Gelator 4. A multifunctional Schiff base with AIEE, Gelation ana mechanochromic properties for anti-counterfeiting applications 5. Discriminative “Turn-On” of Al^{3+} and Ga^{3+} Ions as well as aspartic acid by two fluorescent chemosensors 6. An arene-based chemodosimeter for the ‘Turn-On’ sensing of picric acid. Summary. List of publication.

16. GUPTA (Ruchika)
Band Gap Engineering of Molecular Architectures Based On Metalloligands: Applications In Visible-Light Mediated Catalysis.
Supervisor: Prof. Rajeev Gupta
Th 26586

Abstract

Semiconductor-based photocatalysis is aimed towards the conversion of solar energy into the chemical energy. This strategy is particularly helpful for the production of valuable chemicals and for the degradation of harmful pollutants. The semiconductor-based photocatalysis can be traced back to the discovery of photocatalytic activity of TiO2. However, TiO2 is insensitive to a large portion of the solar energy spectrum, i.e., visible light. To overcome this limitation, research has been focused on developing novel semiconductor materials that can efficiently absorb solar energy in the visible region. Metalloligand-based architectures offer integration of the photosensitive unit (i.e., metalloligand) for light harvesting while secondary metals can act as the reaction centers. Importantly, the electronic characteristics of the resultant architectures can be manipulated by tuning either the primary metal in a metalloligand or secondary metal ions as well as the associated ligands. The aim of the present dissertation is to showcase the significance of metalloligand-based architectures in visible-light driven catalysis. This dissertation is divided into five chapters. Chapter 1 is introductory in nature and discusses the basic principles of semiconductor photocatalysis and provide selected examples of architectures based on metalloligand(s) that have been utilized as the photocatalysts. Chapters 2 and 3 present synthesis of two lanthanide (Ln; Ln = Tb, Eu)-based macrocycles and coordination polymers (Ln-CPs), respectively; synthesized using the strategically designed Co-based metalloligands containing appended arylcarboxylate groups. The Ln-macrocycles exhibited selective adsorption of neutral dyes over both cationic and anionic dyes while also functioned as efficient visible-light-driven photocatalysts for the photodegradation of cationic dyes and a few antipsychotic drugs. In Chapter 3, Ln-CPs were employed for the complete photodegradation of the selected antibiotics. In Chapter 4, a Co-based metalloligand, containing appended arylacrylate groups, was utilized for the synthesis of two Ln-CPs (Ln = Tb, Eu) that were utilized as the photocatalysts for the selective oxidation of a series of alcohols and sulphides to their corresponding aldehydes/ketones/sulfoxides. In Chapter 5, a Co-based metalloligand, bearing an additional arylcarboxylate group in addition to four basal arylcarboxylate groups, was utilized for the synthesis of a Zn-CP. This Zn-CP was employed as an efficient photocatalyst for the photocatalytic oxidation of a variety of hydrocarbons.

Contents

17. JITENDER KUMAR

Optical Nanoprobes for Toxic Ion Sensing and in Vitro Cytotoxicity.

Supervisor: Prof. Indrajit Roy

Th 26587

Abstract

This thesis title “Optical nanoprobes for toxic ion sensing and in vitro cytotoxicity” contains eight chapters. The first chapter introduces the concept of nanoscience and its relevance and significance in the multiple fields, demonstrating the major impact of nanoscale materials in the field of toxic ion sensing and therapeutic applications. The second chapter involves the literature review related to research work carried out inside this proposal. The third chapter discusses the detailed experimental characterization techniques utilized throughout the research work. The fourth chapter is the first experimental part of the thesis, entitled “Rhodamine-B Derivative-linked Upconverting Nanophosphors for NIR stimulated FRET based Ratiometric Detection of toxic Ions”. The fifth chapter comprises a second experimental chapter of this thesis entitled “Synthesis & Characterisation of Eu(III) doped - Downconverting Nanophosphors (GdVO4:Eu3+) and their selective fluorescence response towards Arsenic (III) in water”. The Sixth chapter comprises a third experimental chapter of this thesis entitled “MOF encapsulated Perovskite Nanocrystals (MOF-PNC) for Selective and Ultrasensitive Detection of Mercury (II) ions”. The Seventh chapter comprises a fourth experimental chapter of this thesis entitled “Rose Bengal modified Upconverting nanophosphors for NIR-stimulated Photodynamic therapy”. The eighth chapter is the concluding chapter of all the experimental chapters embodied in this thesis.

Contents

18. JITENDER KUMAR

Study on Sensitivity Enhancement of SAW (Surface Acoustic Wave) Based Chemical Vapor Sensors.

Supervisor: Prof. Vinay Kumar Singh

Th 27078

Abstract

In the current era of accelerated scientific and technological advancement to meet the requirements of the people, an unfavorable side also exists in the form of radiation, chemical and environmental pollution. Toxic gases are being used much more frequently in both domestically and in industries. These chemicals and substances having health-hazard properties such as irritation, sensitization, and carcinogenicity are called hazardous chemicals. There are numerous such chemicals available, and they are classified as Toxic Industrial Chemicals (TICs). Apart from these, there are several chemical compounds specially synthesized for destructive purposes called chemical warfare agents (CWA). These agents are primarily manufactured and used for mass destruction during war. The vapors of these agents are most dangerous to life. Hence, there is an urgent need to develop reliable, selective, fast responding, sensitive sensors to detect these harmful agents for war scenarios as well as homeland security. As a result, extensive research is needed to develop sensitive and effective gas sensors for use in real-world scenarios. Various types of technologies and associated approaches are used to monitor toxic gases and lethal vapors, which include electrochemical sensors, ion mobility spectroscopy, gas chromatography (GC), flame photometric, infrared spectroscopy, semiconductor, photo ionization detector and surface acoustic wave. Gas sensors play a crucial role and help to keep a cleaner environment by giving an early warning of leakage of toxic gases. These types of sensors should be able to provide continuous monitoring of toxic gas, chemical warfare agent or pollutant gases in the environment. To improve response performance, efforts are currently being made worldwide to engineer new sensor materials and innovative sensor mechanisms. Nerve, Blister, Blood and Choking agents having high toxicity comes under the category of CW agents which can harm human body different ways. Hence, there is a serious need for developing such sensors that can give an early alarm about the presence of chemical agents in the environment, particularly when its concentration is as low as parts per billion (ppb) level so that the life of people can be saved. Therefore, there is urgent requirement of sensors such as electronic noses for reliable detection of CW agents in the presence of interferents. Although numerous gas sensing technologies are available these days, Surface Acoustic Wave (SAW) based sensors are preferable because of their high sensitivity, low cost, low maintenance, operation in harsh environment, wireless operation, etc. The SAW technology is a mature technology where electronic signal processing devices such as delay lines, band pass filters, resonators etc., and variety of physical, chemical and biological sensors are developed. Normally, a SAW device has two comb-like metal electrode structures for input and output called inter-digital transducers (IDTs). These IDTs fabricated on piezoelectric substrate by photolithography process. The input IDTs is used as transmitter to convert the electrical signal to SAW, and output is used as a receiver to convert the SAW into an electrical signal. Therefore, IDTs play a key role and used to convert energy from one form to another form by using a piezoelectric substrate. The centre frequency of the device depends on the geometry of electrodes and velocity of the piezoelectric material. The properties of piezoelectric material such as electromechanical coupling coefficient and temperature coefficient of delay are considered very critical parameters for the fabrication of SAW devices. Since the acoustic energy is confined to the surface, perturbations on the surface affect the properties of SAW and this is exploited to realize various types of sensors. In the present study, efforts have been made towards design, development and

the sensitivity enhancement of SAW based sensors which can detect the nerve agents along with VOC's, TICs, and simulants. Since the synthesis of nerve agents is prohibited due to their high toxicity, the present work was carried out with their simulants instead of using the actual CW agent. DMMP (Dimethyl methyl phosphonate), TEP (Triethyl phosphate), DECP (diethyl chlorophosphate) are the well-known simulant of nerve agent and similarly MS (Methyl salicylate), DBS (Dibutyl sulphate), and DCP (1,5 Dichloropentane) were used as simulants of blister/mustard gas. Efforts were also made to improve the selectivity and sensitivity of the SAW based sensor.

Contents

1. Introduction 2. Realization of metal oxide-based SAW-E nose 3.Studies on SAW based Gas chromatography for fast detection of volatile organic compounds 4. Development of highly sensitive SAW-PV A based humidity sensor 5. Sensitivity enhancement study for SAW based chemical sensor. List of publications/Conferences

19. KATHURIA (Ishana)
Synthesis and Applications of Chromogenic Light Controlled Probes.
Supervisor: Dr. Satish Kumar
Th 26588

Abstract

The thesis is concerned with the synthesis, characterization, and analysis of the properties of novel photochromic compounds and their derivatives. It includes six chapters containing the synthesis of photochromic conjugates such as oxazines, spiropyrans, merocyanines and their applications. The photoresponsive molecules were synthesized using optimized processes. The product`s structure and conformation were determined using spectroscopic methods (IR, NMR, HR-MS, and UV-visible spectroscopy), DFT studies and in certain cases, single-crystal X-ray crystallography. To examine harmful ion sensing, UV-visible, digital colorimetric, and fluorescent methods were employed. Dynamic light scattering (DLS) investigations were used to determine the aggregation tendencies. Cyclic voltammetry was also used to study the probes` electrochemical response. Furthermore, computational simulations based on density functional theory were employed to analyze the experimental data and establish the complexity and alteration in structure. Chapter-1 Photoresponsive moieties used in drug delivery systems Chapter-2 Light and redox-sensitive benzothiazolinic-merocyanine salts for the detection of harmful ions in water bodies Chapter-3 Light responsive, electrochemically dimerizable, capture and release device based on photochromic oxazine for detection of Hg2+ ions in different solvents Chapter-4 Derivatives of photochromic nitrooxazine for the detection of toxic ions in aqueous media Chapter-5 Influence of Acid on Ring-Opening, Fluorescence, Aggregation, Electrochemical Oxidation, and C-C bond Coupling of Spiropyran Derivatives Chapter-6 Synthesis and applications of new photochromic thia-oxazine

Contents

1. Photoresponsive moieties used in drug delivery systems 2. Light and Redox sensitive benzothiazolinic-Merocyanine salts for the detection of

harmful ions in Water Bodies 2A.A Substituted benzothiazolinic merocyanine derivative as a reversible, selective, colorimetric and fluorescent probe for the detection of HSO4 - in aqueous solution 2B. A light-responsive, highly sensitive probe to perceive mercuric ions using fluorescence, colorimetric & electrochemical techniques in water, solid-state and biological sample 2C. Colorimetric sensor for the detection of barium metal ion in water 2D. Colorimetric sensing of cyanide anion in aqueous media using merocyanine salt contaning ferocene moiety 2E. Experiemental section Chapter 3. Light responsive, electrochemically dimerizable, capture and release device based on photochromic oxazine for nanomolar level detection of Hg2+ ions in different solvents 4. Derivatives of photochromic nitrooxazine for the detection of toxic ions in aqueous media 4A. Sensing of copper ions in water using spiropyran synthesized via photochromic oxazine and its spin properties in complex 4B. A oxazine – based colorimetric sensor for the detection of Cr3+ and Al3+ in aqueous media 4C. Experimental 4D. References 5. Influence of Acid on ring-opening, Fluorescence, Aggregation, Electrochemical Oxidation, and C-C bond coupling of spiropyran derivatives 6. Synthesis and applications of new photochromic thia-oxazine.

20. KAVITA

Synthesis and Characterization of Novel Sugar based Chalcones, Coumarin-Chalcone hybrids, Coumarin Linked Morpholine Fused Triazoles and Isochroman Fused Coumarin and their Antifungal Activity.

Supervisor: Prof. Brajendra Kumar Singh

Th 27210

Abstract

This thesis contains four experimental chapters. The first experiment chapter titled "A Highly Efficient and Facile One-Pot Synthesis of Novel Glycopyranosyl-4-biaryl Butenone Derivatives". In this chapter, an efficient and facile reaction methodology for the synthesis of 1-glycopyranosyl-4-biaryl butnone has been established starting from different C-glycosides, aryl aldehydes, and aryl boronic acids in 75 - 85% yields via one-pot metal-catalyzed Suzuki-Miyaura coupling/ aldol condensation reaction. The second experimental chapter titled "Synthesis, characterization, and antifungal activity of novel Chalcone-Coumarin hybrid molecules by a triazole linker using a green solvent". In this chapter, the synthesis of the Chalcone-Coumarin hybrid molecules via a triazole linker utilizing low-cost starting materials and by using a green solvent. In this methodology, novel 4-(4-((4-cinnamoylphenoxy)methyl)-1H-1,2,3-triazol-1-yl)-2H-chromen-2-one derivatives have been synthesized using Cu(I)-catalysed click reaction of 4-azido-2H-chromen-2-one with different substituted propargylated chalcones in 77-85% overall yield. The third experimental chapter "Synthesis, characterization, and antifungal activity of heterocycle-linked morpholine fused 1,2,3-triazoles". In this chapter, we sythesised a series of morpholine fused triazoles linked to O-/N-heterocycles utilizing a 1,3-dipolar cycloaddition reaction at room temperature and further evaluated in vitro studies against fungi R. solani. A small series of heterocycles linked morpholine fused triazole have been synthesized using click chemistry and were evaluated for their antifungal activity. Two compounds showed excellent growth inhibition against Rhizoctonia solani. The forth experimental chapter "Synthesis, characterization, and antifungal activity of isochromane fused coumarin". In this chapter, a series of isochroman have been synthesized and these were further evaluated for their antifungal activity against Rhizoctonia solani, a plant pathogen. Some of the synthesized compounds demonstrated strong antifungal efficacy at low doses (10-0.62 µM).

Contents

1. A highly efficient and facile one-pot synthesis of novel sugar based chalcones derivatives 2. Synthesis, characterization, and antifungal activity of novel chalcones-coumarin hybrid molecules 3. Synthesis, characterization, and antifungal activity of heterocycleslinked morpholine fused 1,2,3-triazole 4. Synthesis, characterization, and antifungal activity of isochroman fused coumarins. Summary. List of Publications.

21. KOHLI (Sahil)
Metal Based Nanocomposited for the Green Synthesis of Biologically Active Heterocycles.
Supervisor: Prof. Sunita Hooda
Th 27079

Abstract

Heterocycles are an essential scaffold which has both industrial and pharmacological applications. These can be prepared using wide variety of reaction conditions such as the use of costly catalyst, harmful solvent, and harsh reaction conditions. Although several methods are involved, the chemistry arena is now moving towards the greener way of synthesis. Nanocatalyst plays an important role to achieve such green pathways for the synthesis of heterocycles. This is because the nanocatalysts are highly reactive, selective, and stable; thereby it replaces the conventional catalyst. In present work, the various nanocatalysts has been designed and characterized using various techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM) and so on. The obtained nanocatalysts were further used for the synthesis of heterocyclic motifs such as Xanthene, 1,4-Dihydropyridine, Polyhydroquinoline, 4H-pyran, 2-substituted benzimidazole, 2,3-dihydroquinazolinones, and imidazole derivatives under green reaction conditions.

Contents

1. Introduction 2. Review of literature 3. Aims and objective 4. Preparation of gold-supported NiAITi-layered double hydroxide nanocatalyst and its applications in a one-pot catalytic synthesis of Xanthene, 1,4-Dihydropyridine, Polyhydroquinoline, and 4H-pyrna derivatives 5. AI_2O_3/CuI/PANI nanocomposite catalysed green synthesis of biologically active-2 substituted benzimidazole derivatives 6. A magnetically recoverableFe_3O_4@EDTA/Cul nanocatalyst for the green synthesisss of biologically active 2,3,-diydroquinazolin-4(1H)-ones 7. An efficient and recyclable ZnO/CuI/PPy nanocomposites for the green synthesis of biologically active 2,4,5-trisubstituted imidazole derivatives. Summary.

22. KOMAL

Environmentally Benign Synthesis and Physicochemical Characterization of Silver Nanoparticles: Biomedical & Catalytic Applications.

Supervisors: Prof. Shrikant Kukreti and Prof. Mahima Kaushik

Th 27080

Abstract

The field of nanotechnology is growing continuously due to the rapid emergence of diverse nanomaterials with unique functionality and size-dependent physicochemical properties, which significantly distinguish them from their bulk analogue. Synthesizing materials in the nanoscale dimension constitutes the most exhilarating aspect of nanotechnology. Synthesis of metallic nanoparticles (including gold, silver, zinc etc.) has been a center of focus for researchers and hence is one of the most captivating areas of exploration, due to their employment in a great number of applications like biomedical, medical, electronics, environmental, and molecular biology etc. Due to environmental issues, attention has also been shifted towards green nanotechnology with a central objective of nanomaterial synthesis following an environmentally benign route. Unlike chemical methods, the synthesis of nanomaterials using plants and biological entities like yeast, fungi and bacteria has been manifested as cost-effective, clean and safe. Among the metallic nanoparticles, nanosilver (silver based nanomaterial) has gained a lot of popularity due to its unique biological, chemical and physical properties as compared to its bulk counterpart. Synthesizing silver nanoparticles by conventional methods involves the requirement of (i) an Ag precursor, (ii) a reducing agent and (iii) a stabilizing agent. However, the synthesis of silver nanoparticles employing plants is highly meritorious, as biomolecules act as both reducing and stabilizing agents. Thus, nanoparticles can be synthesized in a facile manner with high stability by following the green or plant based synthesis. In addition to the expanding bio-medical and bio-sensing applications of silver based nanoparticles, their interaction with biological molecules has also become an active area of research in recent years. Such interactions are critically determined by the shape, size and surface functionalization of nanomaterials under study. Investigating the interaction behavior of metallic nanoparticles with nucleic acids enables us to understand their impact on structural integrity, synthesis and replication of DNA and RNA molecules. During this study, silver nanoparticles have been synthesized using Epipremnum aureum (money plant) leaves extract and are studied for their interaction with Calf thymus DNA. Several biophysical and physicochemical methods have been employed to carry out characterization and interaction studies. The unique optical feature is exhibited by the well-dispersed colloidal solution of silver nanoparticles, which depends on the extent of particle aggregations and can be determined by the specific SPR (surface plasmon resonance) profile. The SPR property varies significantly with the particle size, composition, shape, distance among individual particles, and refractive index of the medium. Modulation in color response and SPR band in response to alteration in these factors, laid the foundation of the naked-eye colorimetric sensing procedure. A complete experimental chapter has been devoted to studying the use of plasmonic properties of silver nanoparticles for developing sensing strategies for anticancer drugs and DNA.

Contents

1 Introduction ans review of literature 2. Material and methods 3. Syntheis, characterization and DNA interaction studies of silver nanoparticles synthesized from *Epipremnum Aureum* leaves extract: a physiochemical approach 4. Dye degration potential of tannic acid-mediated silver, gold and palladium catalytic kinetics study based on work function 5. Development of simple and facile colorimetric sensor for successional detection of an anti-cancer drug (Coralyne) and calf-thymus DNA based on aggregation and anti-aggregation of tannic acid-mediated silver nanoparticles 6. Exploring the potential of i-motif structure formed by C-rich DNA sequence for the formation of DNA-templated silver nanoclusters 7. Conclusion. Bibliography. List of publications and conferences.

23. LITTLE

Synthsis, Characterization and Application of Pillared Clay Adsorbents for the Removal of Dyes from Contaminated Wastewater.

Supervisor: Prof. Rajiv Singh

Th 27081

Abstract

The abstract of the thesis entitled "Synthesis, Characterization and Application of Pillared Clay Adsorbents For The Removal of Dyes From Contaminated Wastewater**"** Is To Be Submitted By LITTLE to University of Delhi for the award of Ph.D. Degree in Chemistry. Water is one of the most valuable natural resources on Earth. Due to indiscriminate anthropogenic activities, the problem of water pollution has emerged as a major global concern. Water is contaminated primarily by industrial pollutants of organic/inorganic nature. Synthetic dyes form a major class of such pollutants and many of these dyes are toxic and persistent in nature. These dyes have now become threat to humans as well as the environment. Cationic dyes such as Malachite Green (MG) and Chrysoidine Y (CY) are environmentally persistent and hazardous to humans as well as aquatic life. Various techniques including physical, chemical, and biological methods have been utilized to overcome the problem of water contamination with dyes. Except adsorption, no other technique holds much potential to remove these dyes from contaminated effluents. Adsorbents like bentonite (Bt),which is cheap and abundantly available has been extensively explored for the removal of dyes from water.This thesis mainly focuses upon the synthesis of pillared bentonite based adsorbents in the removal of dyes from contaminated wastewater. The subject matter in the thesis is divided into four chapters. Chapter I deals with the review literature of water contamination, Bt clay, classification of dyes and various dye removal methods. Chapter II describes the process "Pillaring" of Bt clay by polyhydroxy Aluminium (Al), Iron (Fe) and Tin (Sn) chloride. Adsorption capacity of raw-Bt and pillared interlayer clays (PILCs) was examined for two dyes, namely, Malachite Green (MG) and Chrysoidine-Y (CY) from their aqueous solutions. Chapter III deals with the synthesis of pillared clay beads (PCBs) and their application in cationic dye removal. Chapter IV describes the synthesis of pillared clay hydrogels (PCHs) and their application in dye removal from aqueous solutions. These chapters include characterization of modified adsorbents by using X-ray diffraction (XRD), Fourier Transform Infrared spectra (FT-IR), Brunauer-Emmer Teller (BET)

analysis, Thermogravimetric analysis (TGA), and Scanning Electron Microscopy (SEM). The effects of ysicochemical parameters like solution pH, dose, and dye concentration were investigated. The adsorption behavior of the developed adsorbents was studied using various adsorption isotherms, kinetic models and thermodynamic tudies.Thermodynamic studies were performed to determine the adsorption behavior of PILCs and PCBs. studies. The modified adsorbents were also examined for their regeneration potential.

Contents

1. Introduction 2. Aluminium, iron and tin pillared bentonite clay for cationic dye removal 3. Alginate pillared benronite for efficient adsorption of cationic dyes 4. Pillared bentonite hydrogel composites for the removal of cationic dyes. Summary. List of publication.

24. LOCHAB (Amit)
MWCNTs Based Nanocomposites as Electrochemical Sensor for Environmental Applications.
Supervisor: Prof. Reena Saxena
Th 27208

Abstract

This thesis discusses about the synthesis, characterization and fabrication of electrochemical sensors for the determination of various environmental pollutants. There is excessive release of these environmental pollutants into our environment through untreated release of effluents by pharmaceutical industries, factories and through leaching etc. Due to which it imposes serious health concerns for marine life and humans also. World Health Organization (WHO) and United States Environment Protection Agency (USEPA) have set maximum permissible limit for these pollutants for drinking water above which it is unsafe. There is essential need for the determination of these environmental pollutants in natural conditions. For which, there are several techniques available such as Flame Atomic Adsorption Spectroscopy (FAAS), Inductive Coupled Plasma Mass Spectrometry (ICP-MS), High Performance Liquid Chromatography (HPLC) etc. which are cumbersome, costly and require special sampling procedures but on the other hand electrochemical sensors solves not only these problems but are also fast, can perform speciation of analyte and can predict the mechanism. Voltammetry technique in electrochemical sensor have been widely adopted for the determination of both toxic metal ions and organic pollutants like drugs. The working electrode in voltammetry can be made further selective towards the detection of these pollutants by fabricating it with suitable nanocomposites. Here we have synthesized different types of nanocomposites that have been first characterized and then combined to form nanocomposite that is loaded over an ITO (Indium Tin Oxide) electrode. The nanomaterials like MWCNTs, metal oxides, conducting polymer etc. have specific characteristics like high conductivity, surface area and ease in modification that helps in electrochemical determination of these pollutants. Here we have fabricated T-MWCNTs-ITO electrode which have been used for the selective determination of thallium, SnO2-MWCNTs-IL/ITO and MnO2-MWCNTs-IL/ITO for cadmium, Asp-MWCNTs/IL-ITO for paracetamol and diclofenac, Ppy/MWCNTs/IL/-ITO for chloramphenicol.

Contents

1. Introduction 2. Experimental 3. Synthesis, Characterization and Fabrication of Electrodes based on Nanocomposites 4. 3-Amino-1,2,4-triazole-5-thiol Functionalized MWCNTs (T-MWCNTs) based Electrochemical Sensor for Determination of Thallium 5. Metal Oxide and Ionic Liquid based MWCNTs Nanocomposite (SnO2/MWCNTs/IL & MnO2/MWCNTs/IL) as Electrochemical Sensor for Determination of Cadmium 6. Asparagine Functionalized MWCNTs and Ionic Liquid (Asp-MWCNTs/IL) based Electrochemical Sensor for Determination of Diclofenac and Paracetamol 7. Polypyrrole and Ionic Liquid based MWCNTs Nanocomposite (Ppy/MWCNTs/IL) as Electrochemical Sensor for Determination of Chloramphenicol. Summary. List of publications.

25. LOVENEESH KUMAR
Development of Sustainable Catalytic Methodologies for Condensation Reactions: C-C and C-N Bond Formation.
Supervisor: Dr. Rupesh Kumar
Th 27082

Abstract

C-C and C-N bond formation reactions are key phenomenon for any synthetic organic chemistry as it set up the carbon backbone of every molecule by linking smaller molecules to get a complex structure. These reactions are responsible for synthesis of medicines, agrochemicals and molecules of significant importance in materials science. With the rising demands of creating environmentally friendly and reusable energy sources, there is an urgent requirement of generating and adapting green sustainable practises in industry as well as in academic research. Green chemistry is one of the most trending and fascinating branch of science that leads us to sustainable growth of future science and technologies. As a result, numerous methodologies have been reported in the field of organic chemistry based on environment-friendly and energy conserving techniques. Henceforth, creating multifunctional technologies have extreme importance and at same time challenging as well. Therefore, these roles can be achieved using Condensation reactions, Depending upon the requirements, biological molecules of paramount importance can be made using Condensation reactions using a metal catalyst or an organic base. In this work, both the methodologies have been used and molecules of biological significance were synthesized.

Contents

1. Introduction 2. Review of literature 3. Aim and objectives 4. Successive oxidation-Condensation reactions using multifunctionzl gold supported nanocomposite (Au/MgCe-HDO) 5. Microwave assisted catalyst-free multicomponent one –pot green synthesis of highly functionlized aminocyanopyridines and dihydroquinolines in aqua medium and its *In-silico* Studies 6. Development of bioactive 2- substituted benzimidazole derivates by using MnO_x/HT nanocomposite catalyst 7. Applications of MnOx/HT nanocomposite catalyst for the multicomponent knoevenagel tandem reactions 8. Summary.

26. MAMTA KUMARI

Spectroscopic Investigation of Stable and Potent Pyrazole Analogues of Curcumin inside Various Microenvironments.

Supervisor: Prof. Subho Mozumdar

Th 27083

Abstract

Curcumin is a yellow polyphenolic compound present in rhizome of Curcuma longa Linn that furnishes wide range of biological applications such as; anticancer, antiinflammatory, antiantioxidant, cystic fibrosis, anti-Alzheimer's. However, these biological applications are strictly hindered due to the various factors such as; lack of bioavailability that primarily originates from its very low aqueous solubility and also the rapid degradation under physiochemical conditions. The diketo moiety of curcumin is highly responsible for the degradation of curcumin, the and also low average lifetime due to the presence of ESIPT process. In order to achieve maximum biological benefits of curcumin, various efforts has been made by the scientific community in the direction of structural modification in the structure of curcumin. Herein, the β-diketone moiety present in curcumin has been modified into a 5-membered pyrazole ring to form curcumin pyrazole derivative and due to this modification the ESIPT process is highly perturbed. The various biological applications has been reported for these curcumin pyrazole, the fundamental knowledge refarding the photophysics of CPD and CPPD is still limited. In this thesis, the photophysical properties of curcumin pyrazole derivatives (CPD and CPPD) in the presence of different solvent enviornments.Moreover, the aqueous solubility of curcumin pyrazole derivative was found to be enhanced as compared to curcumin but it is not sufficient for the desired efficacy. The work that has been described in this thesis certainly indicates that the limitations associated with curcumin were highly overcomed with the formation of pyrazole derivatives of curcumin and also after the encapsulation of these derivatives inside the various organized assemblies

Contents

1.Introduction and review of literature 2. Characterization techniques 3. Solvent dependent photophysical study of stable and medicinally active diketone modified pyrazole derivatives of curcumin: a spectroscopic study 4. Spectroscopic investigation of interaction of curumin pyrazole derivatives with various surfactants (cationic, anionic and non-ionic) in an aqueous environment 5. Photophysical investigation of interaction of interaction of pyrazole derivatives of curcumin with β-cyclodextrin to from inclusion complexes in an aqueous solution: a spectroscopic study 6. Spectroscopic investigation of interaction of pyrazole derivatives of curcumin with an FDA approved biodegradable polymer named soluplus in an aqueous solution 7. Conclusion. List of publications.

27. MANN (Garima)

Synthesis and Evaluation of Targeted Agents for Imaging and Drug Delivery.

Supervisors: Prof. M. Thirumal and Dr. Anupama Datta

Th 27084

Abstract

Non-invasive imaging techniques have significantly revolutionised diagnostic and therapeutic approaches. Early prediction of drug response, asymptotic and accurate disease diagnosis, as well as monitoring of disease progression, has been made possible by molecular imaging modalities. The term molecular imaging is primarily applied to in vivo detection of cellular interactions via the administration of molecular imaging agents. This visualisation of data provides information on molecular and cellular biological processes which aids disease diagnosis. A sub-pharmacological amount of a tracer when injected distributes within the body according to its biochemistry and provides a detectible signal visualised as a two- or three-dimensional image. Apart from providing information about the functional state of the target organ, molecular imaging also plays a pivotal role in comprehending the drug's mechanism of action, efficiency, and safety parameters.

Contents

1. Introduction 2. Bio-evaluation of ^{99m}TC labelled homodimeric chalcone derivative as amyloid β targeting probe 3. Sythesis and pre-clinical evaluation of ^{99m}Tc labelled chalcone derivative for amyloid β imaging post head trauma 4. Synthesis of mGluR1 targeted mesoporous silica nanoparticles functionalized with methoxy with methoxy phenyl piperazine 5. Synthesis of estrogen targeted nanoparticles for application in theranosis 6. Synthesis of methionine doped graphitic carbon Nitride nanosheets for SPECT imaging. List of publication. List of conferences and presentation.

28. MEENA (Dhan Raj)

Synthesis and Characterization of Pd(II), Ni(II), and Mn(III) Schiff Base Complexes as Catalysts for Organic Transformations.

Supervisor: Prof. Surendra Singh

Th 27211

Abstract

The thesis entitled “Synthesis and Characterization of Pd(II), Ni(II), and Mn(III) Schiff Base Complexes as Catalysts for Organic Transformations” is consisted by five chapters. Chapter first includes the basic information about catalysis, Schiff bases, metal (Pd, Ni, Mn) complexes of Schiff bases, Mizoroki-Heck reaction, Suzuki-Miyaura reaction and homocoupling reaction of phenylboronic acids. The chapter also includes the literature summary of approximately last ten years of catalytic systems used in above mentioned coupling reactions with the applications of coupling products of these reactions. Chapter second consisted of the synthesis and characterisation twenty-one Schiff bases and their Pd(II) complexes. These Schiff bases and complexes were characterized with various instrumental techniques like NMR, FT-IR, HRMS, UV-Vis, CHNS analysis, TGA and single crystal XRD. We did the study of formation of cis- and trans- geometrical isomers of these palladium (II) complexes. The synthesized Pd(II) complexes was found catalytically active towards Suzuki-Miyaura reaction between aryl halides and styrene’s in DMF solvent at 140°C temperature in the presence of NaHCO3 base. The afforded catalytic coupling product was found in moderate to excellent yield using 5 mol% of Pd(II) complexes. Third chapter deals with the Suzuki-Miyaura reaction catalysed by N,O- donor Pd(II) Schiff bases complexes. The chapter includes the deep study of optimization of reaction conditions and the electronic and steric effects responsible for the activity of Pd(II) complexes. The steric and electronic effects on phenylboronic acid for the formation of coupling products with aryl halides were also studied and corresponding 43 substrates were synthesized and characterized by 1H-NMR and 13C-NMR spectroscopies. Chapter fourth consisted with the synthesis and characterisation of polymeric Mn(III) Schiff base complexes and their application in selective oxidation of primary alcohols. Chapter fifth deals with the synthesis and characterisation of Ni(II) complexes and their utilization in carbon-carbon homocoupling of phenylboronic acids.

Contents

1. Introduction 2. Synthesis and structural studies of Pd(II) complexes of bidentate Schiff bases and their catalytic activities as precatalysts in the Mizoroki-Heck re 3. Suzuki-Miyaura cross-coupling reaction catalyzed by Pd(II) complexes of N,O- donor Schiff base ligands 4. Reusable Polymeric Mn(III) Salen complexes as efficient catalysts for the selective oxidation of primary and secondary alcohols 5. Synthesis and characterization of Ni(II) Schiff base complexes and their catalytic activities as homogeneous catalysts for carbon-carbon homocoupling of phenyboronic acids. Summary. List of publications.

29. MEENA (Priyanka)
Base-Mediated Chemo- and Regioselective Intermolecular Hydroamination and Methylsulfinylation of Alkenes.
Supervisors: Prof. Akhilesh K. Verma and Dr. Akhilesh Bharti
Th 27085

Abstract

We have developed an efficient, metal and protection-free protocol for the synthesis of highly functionalized N- and S- containingmoieties *via* in situ generation of amines and methyl sulfinyl compounds with excellent regioselectivity from easily accessible starting material. The developed synthetic method also allows for the synthesis of free (NH) of 2-amino heterocyclic under a metal-free condition base-promoted intermolecular anti-Markovnikov hydroamination reaction of functionalized aminopyridine and styrenes via a radical pathway forming products in good to excellent yields. The protocol is atom economical and environment-friendly and has been successfully extended for hydroamination of aminoquinoline, aminopyrimidine, aminopyrazine, and benzylaminopyridine with alkenes. The versatility of the reaction has been demonstrated by performing controlled mono- and bis-hydroamination reactions of 1,3-divinylbenzene and pyridine-2,6-diamine. Selective hydroamination of divinylbenzene and di-aminopyridines leaving vinyl and amino groups intact that could be further used as a handle for various functionalization.Further, we have described a transition-metal-free KOH-mediated approach for the direct nucleophilic addition of *N*-Heterocyclic secondary amines onto alkenes have been developed. It was established that hydroamination of aromatic alkenes with secondary amines can be utilized for addition reaction. Mild reaction condition was also tolerable to a diverse set of benzylaminopyridine substrates. The methodology was capable to perform modification in biologically active drug molecule as well as amino acid. Furthermore, we have developed a practical protocol for the transition-metal-free synthesis of a new, highly efficient protocol for the regioselective and direct methylsulfinylation of a wide variety of styrenes under very mild reaction conditions. DMSO along with a simple base was used as a surrogate of the methylsulfinyl group. Developed methodology accommodates various functional groups and affords the methylsulfinylated products in good to excellent yield. Synthetic elaboration of the reaction has been demonstrated by performing controlled mono- and bismethylsulfinylation of 1,3-divinylbenzene. The control experiment and isotopic labeling experiment support the proposed mechanistic pathway.

Contents

1. A brief introduction to hydroaminationand methylsulfinylation chemistry 2. Transition-metal-free regioselective hydroamination of styrenes with amino heteroarenes 3. Base-mediated anti-markovnikov intermolecular hydramination of styrenes eith N-heterocycles secondary amines 4. Transition-metal-free anti-markovnikov intermolecular methylsulfiny of styrenes. Summary of the work.

30. NIDHI
Design, Synthesis and Biological Evaluation of Newer Isatin and Dihydropyridine Scaffolds.
Supervisor: Prof. Rakesh Kumar
Th 27086

Abstract

This thesis is divide in to four chapters, i.e. chapter 1, briefely describe the literature survey about the recent advances in the field of biological evaluation of heterocyclic scaffods such as isatin, dihydropyridine and 1,2,3-triazole derivatives Chapter 2 deals with the synthesis of novel triazole linked 1,4-dihydropyridine-isatin scaffolds as potent anticancer agents and their molecular docking studies Chapter 3 deals with the synthesis of newer isatin-pyrano[2,3-c] pyrazolone Schiff bases as α-glucosidase inhibitors chpter 4, deals with synthesis and bio-evaluation of newer tetrahydropyridines and dihydropyridines based azasugar glucomimetics.

Contents

1. Introduction 2. Sythesis and molecular docking analysis of novel tiazole linked 1,4-dihydropyridine-isatin scaffolds as potent anticancer agents 3. Design and synthesis of newer Isatin-pyrano[2,3,-c] pyrazolone Schiff bases as α-glucosidase inhibitors 4. Synthesis and bio-evaluation of newer tetrahydropyridlines and dihydropyridines based azasugar glucomimetics. Summary.

31. NIRBHAYA (Vishakha)
Development of Carbonaceous Nanomaterials Based Biosensors For Swine Flu Detection.
Supervisors: Prof. Ashok K. Prasad and Dr. Suveen Kumar
Th 27098

Abstract

Nanomaterial defined as materials having a dimension in 1 to 100 nanometer (nm) range. They behave differently from their bulk counterparts due to their high surface area to volume ratio and dominance of quantum effects. In the development of biosensors, nanomaterials play significant role, they act as efficient immobilization matrices owing to their excellent electronic, mechanical, optical, magnetic, and thermal properties. Various types of metals and metal-based nanomaterials like oxides, sulphides, selenides, carbides etc. have been widely employed in the successful development of biosensors. However, these metals based nanomaterials are synthesized from expensive and high molecular weight hazardous precursors. Also, many of these metal compounds tend to agglomerate and may lose their dispersion properties. This difficulty has been overcome by the use of carbonaceous nanomaterials like graphene and its analogs viz. graphene oxide, multi-walled carbon nanotubes (MWCNTs), carbon nanofibers, porous carbon etc. which possess better dispersing ability and comparatively require non-toxic precursors. These nanomaterials exhibit excellent electron transfer properties, high mechanical strength, astonishing electrical and thermal conductivity with excellent biocompatibility. Considerably, graphitic carbon nitride (g-C3N4) nanomaterials are burgeoning semiconductor polymeric materials with bandgap of 2.7 eV, a high N:C ratio (= 3:4) with a small amount of hydrogen and its structure varying from polymer to graphitic. The name "graphitic" is inherited by graphite, as it has a stacked structure with weak van der Waals forces between layers, also recognized as sp2-hybridized graphene replaced by nitrogen. It possesses a porous framework with electron-rich properties, along with basic surface functionalities that help in the facile biofunctionalization of the compound. Nevertheless, its biocompatibility, physicochemical stability, environmentally friendly and economic availability align it towards biomedical applications such as biosensors, therapeutic applications, bioimaging, and antibacterial applications. On the other hand, an analogous material, porous carbon is also a potential nanomaterial owing features such as high effective surface area, pore size distribution and wide pore volume, good conductivity, low-cost, environmental benign, chemical stability and high electrochemical stability, and have tremendous application in electrocatalysis, energy storage, capacitor devices and shows excellent biocompatibility as well as electrical conductivity. Comprehensively, for biosensing aspects nanomaterial as transducer material show distinct features such as efficient immobilization matrix for biomolecules (i.e., antibodies, proteins, bioactive molecules, peptides, and oligonucleotides) conjugation, signal amplification, mediators, electroactive species, and detection probe.

Contents

1. Introduction and literature review 2. Experiemental and instrumentation 3. Nanostructured mesoporus carbon based biosensor for swine flu detection 4. Graphitic carbon nitride nanoflakes based biosensor for swine flu 5. Phosphorus doped graphitic carbon nitride based biosensor for swine flu detection 6. Poly (5-aminoindole) modified phosphorus doped graphitic carbon nitride based biosensor for swine flu detection 7. Summary and future prospective. References.

32. NUTAN RANI

Synthesis and Characterization of Zinc Oxide Nanoparticles for *In Vitro* and *In Vivo* Studies.

Supervisor: Prof. Kalawati Saini

Th 27087

Abstract

The thesis is divided into seven chapters: Chapter 1: Introduction Chapter 2: Characterization techniques Chapter 3: *Azadirachta indica* leaf extract mediated biosynthesized zinc oxide nanoparticles for *in vitro* anticancer study on human lung cancer (A549) cell lines. Chapter 4: *Azadirachta indica* leaf extract mediated biosynthesized zinc oxide nanoparticles for *in vitro* anticancer study on cervical squamous carcinoma (SiHa) cell lines. Chapter 5: Biosynthesis of hydrophilic zinc oxide nanoparticles using *Plumeria obtusa* and *Tabernaemontana divaricata* flower extract for antidiabetic treatment. Chapter 6: Characterization and investigation of antioxidant and antimicrobial activity of zinc oxide nanoparticles prepared using the leaves extract of *Nyctanthes arbor-tristis* Chapter 7: Conclusion.

Contents

33. MISHRA (Anupam)

Design and Synthesis of Peptides Containing Guanidine Amino Acid Analogs for Biological Applications.

Supervisor: Prof. S.K. Awasthi

Th 26590

Abstract

This Research involves the design and synthesis of some novel unnatural guanidine amino acids analogs and their peptide with the help of Solid phase peptide synthesis by Boc, Fmoc, Cbz and tosly protecting groups to create new generation antimicrobial peptides (AMPs) by introducing the cationic group (Guanidine) on the peptide backbone instead of the side chain, this strategy would enhance Drug Delivery and antimicrobial activity. So, I have developed a method for the synthesis of novel unnatural amino acids, yielding peptides with a novel moiety on the peptide backbone, yielding a net positive charge on the peptide backbone. So, I developed three methods of producing cationic backbone peptides. Now we check the Nucleic acid delivery using guanidine backbone peptides. All synthesized peptide has good Electrophoretic Mobility Shift Assay for pDNA (Plasmid DNA) and FAM-labeled oligonucleotides. Also, I performed the pDNA and

oligonucleotide transfection efficiency and we found that C4 24-mer has 80% and C6 24-mer has 50% transfection efficiency respectively. Further to check the antimicrobial activity of synthesized Guanidine backbone peptides. These compounds involve initial binding to negatively charged phospholipids or lipopolysaccharides on the bacterial membrane to create pores resulting in leakage of cellular components and cell death, they are less prone to bacterial resistance mechanisms. Most of the peptides synthesized exhibit potent antimicrobial activity against Gram-positive (Staphylococcus aureus) and Gram-negative (Escherichia coli) bacterial infections. The lead peptide are C6 24-mer which has MIC of 10μg/mL against E. coli and 16μg/mL against S. aureus C3 24 mer. I also synthesized a simple pyrene-modified AIE active Schiff base a fast, sensitive, and thermally stable receptor for fluorescence detection of volatile HCl gas.

Contents

1. Design and synthesis of novel unnatural guanidine amino acid analogs and their peptidomimetics 2. Cellular uptake and nucleic acid delivery using guanidine backbone peptides 3. Antimicrobial activity and cytotoxicity of synthesised guanidine backbone peptides 4. Highly efficient guanidine functionalised sulfonic acid fabricated cobalt ferrite magnetic nanoparticles for clean and scalable synthesis of dihydro quinazolinones product 5. Simple pyrene modified AIEE active Schiff base a fast, sensitive, and thermally stable receptor for fluorescence detection of volatile HCl gas. List of publications. List of conferences and seminars

34. MD SHOAIB
Structrual Diversity and Recognition of Oligopurine-Oligopyrimidine Motif Located at Coding Region of Human *DACHI* Gene.
Supervisor: Prof. Shrikant Kukreti
Th 26589

Abstract

The most significant source of understanding the fundamental principles underlying human existence is the comprehension of the double helical structure of DNA. Various biological functions of DNA are largely dependent on its inherent flexibility as a molecule. It is known to exhibit structural polymorphism giving rise to some extremely significant structural properties. Since the earliest investigations into the structure of nucleic acids, it has been recognized that DNA may adopt helices with than two strands. Such multistranded nucleic acid structures have attracted new attention over the past few decades. The quest results from the in vivo evidence and functional roles of multistranded DNA structures and potential use in therapeutics. Various DNA sequences have a tendency to adopt peculiar hydrogen bonding and structural conformations. Oligonucleotides may undergo folding or join three or four strands of DNA to form multistranded helices such as triplexes or G-quadruplexes. Numerous technological and medicinal uses, such as antisense and antigene techniques, artificial nucleases, array scaffolds, etc., have shown the plethora of multistranded DNA conformations accessible. Oligopurine oligopyrimidine motifs are significantly widespread in mammalian genomes, generating speculation on their potential functions. These tracts have been noted to encourage DNA recombination and decrease DNA replication and transcription. These sequences may take various unusual conformations for example, intramolecular (H-DNA) or intermolecular triplexes upon third strand binding. Triplex-forming oligonucleotides exhibit the great potential to outcompete various DNA binding factors for gene regulation in a sequence-specific as well as site-specific manner. They provide the ability to selectively control homologous recombination processes, mutagenesis, and targeted genomic modification. This approach of gene regulation via genome targeting has also proved to be a useful notion in cell studies where local mutagenesis takes place in TFOS regards. However, the presence, function, and interactions of DNA triplex with systemic proteins need further investigation. The limited stability of these structures might restrict their use in biological systems. Developing ligands that can specifically bind and stabilize DNA triplex is one method for improving their stability. This study demonstrates the formation of parallel intermolecular triplex at human genomic targets. Furthermore, we attempted to study the stabilizing effects of natural alkaloids on DNA triplex G-quadruplex presents another family of multistranded DNA structures that have been proven relevant in biological contexts. Several experimental shreds of evidence clearly demonstrate that G-quadruplex forms in important regulatory regions throughout the human genome. Computational predictions and bioinformatic analysis have suggested that there are more than 300,000 G-rich sequences in the human genome likely to form G-quadruplex structures. The empirical data has indicated that promoters of oncogenes are abundant in putative G-rich sequences compared to rest of the genome. Thus, G-quadruplex may be potentially used as diagnostics and therapeutics in various cancers. This study contains an investigation of the stabilizing effects of alkali metal ions on G-quadruplex formation at the genomic location. Using the current body of knowledge on multistranded structures and their targeting with ligands for therapeutic intervention, the present study is an attempt to better understand how genomic sequences, such as homopurine-homopyrimidine and GC- rich segments of transcription elements of the human genome, generate multistranded DNA structures at specific genomic regions. Bioinformatic tools were used to uncover the biological significance of the sequences involved in the study. The structural characterization of the motifs formed was carried out through biochemical and biophysical techniques such as Gel electrophoresis, UV-thermal denaturation, Circular Dichroism, CD-melting, UV-Visible absorption, and fluorescence spectroscopy.

Contents

1. Introduction and literature review 2. Material and methodologies 3. Sequence-specific recognition of a coding segment of human *DACHI* gene via short pyrimidine/Purine dexyoligonucleotides 4. Alkali cation-mediated topology displayed by an exomic G-rich sequence of TRPAI gene 5. Recognition of *DACHI* triplex with natural alkaloids 6. Conclusions. Bibliography. Publications. Conferences & workshops.

35. NISHU

Structural Polymorphism of Quasi-Palindromic and G-Rich Sequences Present at Genomic Locations and Recognition of G-Stretches by Mitoxantrone.

Supervisor: Prof. Shrikant Kukreti

Th 26591

Abstract

DNA contains the genetic information that allows all forms of life to function, grow, and reproduce. DNA double helical structure was discovered by James Watson and Francis Crick in 1953, and this discovery proved to be a milestone in the history of science. Although a right-handed double helix is the canonical image of a DNA, it has long been recognized that the molecule can adopt many other biologically important non-B DNA structures using non-Watson-Crick and Hoogsteen base pairing. Polymorphism in structural genes in human is a well-known phenomenon which has been utilized for many types of genetic analyses. Structural Polymorphism of DNA is governed by several factors like base sequence, concentration of the cation, pH of the solution, temperature, and other solvent conditions, in which transition from one conformation to another can take place. The advent of human genome has led to a manifold increase of information in nucleotide sequence databases. There are various types of repetitive sequences. including dinucleotide repeats, triplet repeats, and telomeric sequences. The most important aspect of DNA structural and conformational variations is likely to be found in the mechanics of molecular recognition and manipulation by proteins, as they are required to recognize the DNA structure to carry out their function. The enrichment of guanine-rich sequences at various genomic locations such as promoters, telomeres, and hot spot regions, has proved the substantial role of the G- quadruplex in the regulation of gene expression. DNA methylation at such sites is vital and dynamic regulator of transcription, although aberrant methylation has been associated with development of diseases. The sequences, which consist of unsymmetrical inverted repeats, are usually known as quasi-palindrome or imperfect palindrome. Inverted repeats or palindromic sequences are prone to transform into recognized secondary or tertiary structures, such as hairpins, internal loops, bulges, four-way Junction type DNA, and cruciform structures. Generally, inverted repeats are found at the origin of DNA replication or near putative control regions of genes. These unusual DNA structures play important biological roles by offering binding sites for various proteins and help in the regulation of many cellular processes. The studies of DNA and its interaction with drug molecules have been of profound interest, as these serve the purpose to understand and design a new molecule for better efficacy. Several biochemical and biophysical techniques like Gel electrophoresis, UV-thermal denaturation, Circular dichroism, UV-Visible absorption, and Fluorescence spectroscopy have been employed to carry out the structural characterization and the interaction studies.

Contents

36. PAL (Sachin)
Solid State Chemistry of Layered Oxides and Their Structure Property Relationships.
Supervisor: Prof. Sitharaman Uma
Th 27088

Abstract

The synthesis and characterization of new solid-state compounds accompanied by the understanding of the structure-property relationship is the proverbial route to identify novel functional materials. The understanding of the basic solid state chemistry aspects has been useful to design materials with interesting ionic, electronic magnetic, optical, non-linear, multiferroic, and ferroelectric properties thereby leading to their applications. Particularly the layered (two-dimensional) structures have proven to be useful because of the reduced dimensionality. In this context, the present thesis describes the results obtained by the multi-cationic substitutions in the layered perovskite structures, followed by careful study of the altered crystal structures and the subsequent modifications of their physical properties. Lithium based mixed metal oxides possessing the layered honeycomb and layered double hydroxides (LDH) structures have also been considered towards this purpose. A short summary of each chapter is described below. Chapter 1 gives a brief review of the background literature related to the present research work. Specifically, the structural aspects of the various layered perovskite structural families, their significance as functional materials and the need for the exploration to identify new polar structures have been described. The importance of the layered honeycomb mixed metal oxides containing lithium with interesting structural and magnetic properties has been outlined. The details pertaining to the lithium based LDH have been discussed briefly. Chapter 2 is divided into three sections describing the research work on the Dion-Jacobson (DJ) layered perovskite oxides obtained by the incorporation of rare earth ions.2 Chapter 3 deals with the recognition of new DJ layered perovskite oxides obtained as a result of introducing cations such as Bi3+, Pb2+, and Cd2+ ions. Chapter 4 describes the research work done related to the Li+ containing layered honeycomb and layered double hydroxides (LDH). Chapter 5: In this chapter, the overall conclusions of the work presented in the thesis is summarized. The scope for future research towards the development of solid-state materials for potential practical applications are mentioned.

Contents

1. Introduction 2. Identidying new rare earths containing dion-jacobson family of layered perovskite oxides 3.Studying the effects of incorporation of $Bi^{3+,}$ $Pb^{2+,}$ and Cd^{2+} ions in the dion-jacobson layered perovskites 4. Lithium containing layered honeycomb oxides and layered double hydroxides. 5. Conclusion and future directions. List of publications.

37. PARIHAR (Harish)
Cobalt (II) Catalysed Directed C−H Functionalization/Annulation of *N*-Arylguanidines with Alkynes/1,3-Diynes.
Supervisor: Prof. Natesan Thirupathi
Th 26592

Abstract

A family of N,N`-diaryl-N``-(quinoline-8-yl)guanidines were prepared by two methods and these guanidines were subjected to Co(II) catalyzed C-H functionalization/annulation with terminal and internal alkynes under mild condition to afford a family of indole guanidines. Substrates with a range of electronic and steric properties were tolerated. The fluxional behaviour of two guanidines and molecular structures of nine compounds determined by single crystal X-ray diffraction (SCXRD) are reported. Several key experiments were carried out to support the proposed mechanism of alkyne annulation. 8-Aminoquinoline directed N-arylguanidines were subjected to cobalt(II) catalysed C-H functionalization/1,3-diyne annulation to afford 2-alkynalated indole-guanidines in moderate to good yields. Among the various Co(II) sources screened, CoSO4.7H2O turned out to be the best catalyst. The scope of guanidines with 1,3-diphenyldiyne and 1,3-dicyclopropyldiyne were explored. The new compounds were characterised by IR, multinuclear (1H, 13C and 19F) NMR spectroscopy and HRMS. Molecular structures of five new compounds were determined by SCXRD. Competition and labelling experiments were carried out to support the proposed reaction mechanism. Mono-annulation of four N,N-diaryl-N-(quinolin-8-yl)guanidines was carried out with 1,3,5-tris(trimethylsilyl) ethynyl)benzene under milder condition using CoSO4.7H2O as a catalyst. Bis-annulation of monoannulated product was achieved by treating it with one equivalent of guanidine. Molecular structures of three compounds were determined by SCXRD.

Contents

1. Introduction 2. Result and discussion 3. Supporting information 4. Appendix. Synopsis. Abstract.

38. PRITI RANI

Cross linked derivatives of chitosan and magneto chitosan for adsorption of Cd(II), Ni(II),Zn(II) and Pb(II) from wastewater.

Supervisor: Prof. A.K. Prasad and Prof. P.S. Jassal

Th 27090

Abstract

In this research work, the toxic heavy metal ions viz. Cd(II), Ni(II), Zn(II) and Pb (II) were successfully removed from the waste water through the process of adsorption by modified magnetic chitosan beads by cross-linking with glutaraldehyde (GLU), epichlorohydrin (ECH) and ethylene glycol diglycidyl ether (EGDE) etc. The magnetic chitosan beads and its cross-linked derivatives were characterized by using FTIR, XRD, TGA, DTG, DSC, SEM and EDX techniques. FTIR spectroscopy confirms the magnetic property of modified chitosan due to the presence of (Fe-O) bond peaks at 618 cm-1 and XRD confirmed the crystalline behavior of modified magnetic chitosan beads by the presence of sharp peaks. TGA/DTG and DSC thermal analysis that monitor the physical and chemical change and found that the thermal stability were increased with cross-linking of chelating groups with magnetic chitosan. From the scanning electron microscopy, visualizes the morphology and surface structure and found that pore diffusion occurred on the surface and facilitated for the adsorption of metal ions. The EDX analysis carried

out elemental compositions present in adsorbent. Adsorption studies were performed in batch system and evaluated the effect of adsorbent dose, pH of the solution, temperature and contact time. The equilibrium data were well described by Langmuir and Freundlich isotherm models for both magnetic and cross-linked magnetic chitosan beads. The maximum adsorption capacity (qmax) of MCSB and cross-linked MCSB for heavy metal ions was carried out. Comparative kinetic and thermodynamic studies of heavy metal ions on cross-linked magnetic chitosan beads were successfully done.Thermodynamic studies revealed the adsorption process was endothermic or exothermic in nature for the adsorption of heavy metal ions and also tell about the feasibility of the process by the vant'Hoff plot. The maximum adsorption capacity of cross-linked magnetic chitosan beads was calculated by the EGDE-MCSB as compared to GLU-MCSB and ECH-MCSB. Desorption studies carried out with 0.1M EDTA solution to regenerate the adsorbents for further use.

Contents

1. Introduction 2. Review of the previous work 3. Scope and object of the present work 4. Materials and methods 5. Kinetic and thermodynamic studies of Ni(II) ions gluaraldehyde cross linked magnetic chitosan beads 6. Comparative studies on the adsoption of Zn(II) metal ions on its cross-linked epichlorohydrin magnetic chitosan beads 7. Magneticiedge crossilinked chitosan beads as a adsorbent for the removal of Pb(II) ions form Aqueous solution 8. Adsorption of mixture of Cd(II),Zn(II) and Pb(II) ions on magnetic chitosan beads: equilibrium isotherm studies. Summary. List of publications. List of conferences.

39. Ram Sunil Kumar Lalji
Chalcogenation of Quinoxalinones and Benzoxazines using Rhodium and Palladium Catalysts.
Supervisor: Prof. Brajendra Kumar Singh
Th 27212

Abstract

This thesis is divided into three chapters. The work presented in Chapter 1, entitled 'Recent advances in chalcogenation via C-H activation' describes the selenylation and sulfenylation of the organic moieties during the last decade by C-H activation. Chalcogenation refers to the process of introducing chalcogen atoms such as sulfur and selenium to the organic compounds. Sulfur is essential constituent of plants and animals. It has wider applicability in terms of medicines, agrochemicals, food industry, batteries among others. Similarly, selenium is essential for certain enzyme activities, Many biomolecules contain different forms of selenium. The selenium containing drug ebselen has been explored widely by the chemists due to its medicinal properties such as anticancer, antioxidant and anti-HIV among others. Owing to these factors the two chalcogens are very important to the chemists. The work presented in Chapter 2, entitled 'Rhodium-catalysed sulfenylation and selenylation of quinoxalinones 'on water,' describes the selenylation and sulfenylation of quinoxalinones. In the present investigation dichalcogenides have been employed to prepare fourteen selenylated products, eighteen sulfenylated products and four chalcogenation reactions of the potential drug candidates has been performed. To establish the plausible mechanism, control experiments were performed. Further the H/D exchange and deuterium kinetic studies were performed. The formation of the chalcogenated quinoxalinone products were confirmed by their NMR (1H and 13C) spectroscopy, mass spectrometry. The work presented in Chapter 3, entitled "Palladium-catalysed sulfenylation and selenylation of benzoxazines" describes the C-H activation and C-chalcogen functionalisation of benzoxazines. In the present investigation a multitude of dichalcogenides have been employed to prepare 16 sulfenylated products, eight selenylated products, and three organic moieties were chalcogenated as application. Further the H/D exchange, kinetic studies using intermolecular competition reactions were performed. The chalcogenated 3,4-dihydro-1,4-benzoxazine products were confirmed by their NMR (1H and 13C) spectroscopy, mass spectrometry.

Contents

40. RANA (Pooja)

Ultrathin Hexagonal Boron Nitride Nanosheets Based Architectures For Catalyzing Cycloaddition for Catalyzing Cycloadditon and Multicomponent Reactions.

Supervisor: Prof. R.K. Sharma

Th 27091

Abstract

In recent years, astonishing advancements have been witnessed in the rational design and fabrication of well-defined, highly active and selective structured materials for diverse catalytic applications. The prospects of tuning the catalytic properties of nanomaterials by controlling the structural aspects of nanoparticles and manipulation of interaction between the catalytically active species and its support matrix has aided in the engineering of new type of hybrid multifunctional materials that can be deployed for diverse industrially significant organic transformations. A plethora of solid-supported catalytic system have been fabricated so far amongst which two-dimensional nanomaterials analogous to graphene like nanostructures especially, ultrathin hexagonal boron nitride nanosheets has captivated enormous interest owing to their exceptional structural and morphological features such as large surface area to volume ratio, high oxidative resistance, excellent thermal, chemical and mechanical strength, nanometer size, capability of dissipating heat in exothermic reactions and coordinatively unsaturated active sites. In addition, anchoring of superparamagnetic iron oxide, particularly ferrite nanoparticles onto the boron nitride support not only enhances number of accessible active sites for further modification but also endows facile separation via the aid of external magnet and thus emerged as a greener alternative route to energy demanding techniques. Inspired by abovementioned phenomenon attributes exhibited by hexagonal boron nitride layered nanostructures, we have successfully fabricated BN nanosheets based catalytic system and exploited them as promising platform to deliver a wide array of pharmacologically and

biologically significant organic compounds which include synthesis of highly privileged heterocyclic 5-substituted 1H-tetrazoles via [3+2] cycloaddition of sodium azide and nitriles, one-pot multicomponent condensation reaction to yield 3,4-dihydropyrimidin- 2(1H)-ones/thiones, 2-amino-4H-benzopyrans and 1,4-dihydropyridine derivatives

Contents

1. Introduction 2. Theoretical aspects of instrumentation techniques 3. Enhanced catalysis through structurally modified Hybrid 2-D boron Nitride nanosheets comprising of complexed 2-hydroxy-4-methoxxy benzophenone 4. Magnetic boron nitride nanosheets decorated with cobalt nanoparticles as catalyst for the synthesis of 3,4-dihydropynimidin-2(1*H*)-ones/thiones 5. Magnetically responsive two-dimensional boron nitride nanostructured based copper catalyst in the one-pot multicomponent synthesis of 2-amino-4H-benzopyrans 6. Insights into the catalytic potential of rationally designed magnetic boron nitride nanosheets supported Nickel Catalyst for the efficient synthesis of 1,4-dihydropyridine derivatives. Summary. Spectral data. List of publications.

41. SARMA (Liza)

Graphittic Carbon Nitride (g-C_3N_4) Nanocomposites: Synthesis, Characterization, Photocatalytic and Catalytic Applications for Water Remediation

Supervisor: Prof. M. Thirumal

Th 27093

Abstract

Water is indeed the most precious and a basic element for all forms of life on the earth. Unfortunately, water scarcity has become a global challenge and critical in 21st century. Out of 70% of the earths water, 97.5% is saline water and only 2.5% of freshwater is actually available for use. Water pollution, population increase, climate change creates additional pressure on freshwater availability. Water pollution in particular have become an urgent and a realistic problem all over the world. With thousands of industrial chemical wastes, the contamination on water bodies become a key environment trouble. Human activity and industrialization were mounting a huge number of pollutants such as dyes, pharmaceutical such as antibiotics, pesticides, phenols, fluoride, insecticides and detergents. Due to this, more than 780 million people around the globe lack safe potable water. By employing a renewable and abundant solar energy, semiconductor based photocatalysis is considered to be an efficient method for the remediation of environmental pollution. Semiconductor photocatalysis can utilize natural solar light for elimination of numerous organic pollutants without using any kind of additional chemical reagents or external energy. Visible light and solar powered photocatalysis promises fabrication of next-generation materials and hence providing a sustainable water treatment process. To date, various semiconductor photocatalysts such as metal oxides, sulfides and metal free photocatalysts have been used for effective pollutants eradication. It was Fujishima and Honda's invention of TiO2 photocatalysts used as a water splitting in 1972, who created a benchmark and became a popular photocatalyst. However, TiO2 has a wide band gap (~3.2 eV), and absorption takes place only in the UV region which accounts

less than 5% of the whole solar spectra and therefore restricted its use due to lower photodegradation activity in visible light irradiation. Graphitic carbon nitride (g-C3N4), a metal-free, graphite analogue polymeric semiconductor was widely developed and captivated intensive attention owing to its propitious properties. Graphitic carbon nitride (g-C3N4) was first developed by Wang *et. al.* in 2009 as a π-conjugated metal free photocatalyst for water splitting to generate H2 as a future energy fuel. It is nontoxic, highly stable and low cost photocatalysts that can not only protect our environment but can also be used for generation of energy. g-C3N4 can be prepared easily from cheap precursors such as melamine, urea, thiourea etc. via solid state synthesis. Therefore, graphitic carbon nitride (g-C3N4), a novel n-type semiconductor, with outstanding chemical and thermal stability, tunable band gap (2.70 eV) and adjustable electronic structure, has attracted much growing attention as a photocatalyst for various catalytic and 2 photocatalytic applications. Among a range of applications, the recent interest has aroused concern in water cleansing process and utilizing graphitic carbon nitride (g-C3N4) is considered to be a potential candidate as a metal free photocatalyst on large scale water treatment process. However, apart from having such attractive properties, g-C3N4 possess some drawbacks that reduces its application as a photocatalysts. Lower capability of visible-light absorption, recombination of electron-hole pairs and comparative lower specific surface area are some of the shortcomings that limits its performance. To overcome such issues, many efforts have been made by researchers, for instance, doping (elemental and molecular), exfoliation to 2D nanosheets, formation of composites or designing heterostructures with other semiconductors or morphological modifications etc, are some of the successful approaches. After an extensive literature review and motivated from the strategies followed, our sole objective is to design a novel g-C3N4 based photocatalysts with enhanced visible light photocatalytic activities. We have also investigated the catalytic behaviour with NaBH4 in absence of any light to study their performance as a heterogeneous catalyst for nitrophenol reduction and dye degradation. Apart from constructing heterojunction and composites, we have also modified the morphology and understand their mechanism of texture designing. We have further devoted time to elucidate the basic mechanisms during the photocatalytic and catalytic degradation of organic pollutant. We have mainly focused on degradation of dyes and antibiotics, and reduction of nitrophenol. To the best of our knowledge, all the prepared catalyst are novel and there is no such work reported till date.

Contents

42. SEHRAWAT (Hitesh)

Develeopment of Chemotherapeutic Agents: Noscapine Based Ionic Liquids.

Supervisor: Prof. Ramesh Chandra

Th 27092

Abstract

Noscapine having various pharmacological uses as anticancer drug has evolved as a potential chemotherapeutic agent. The anti mitotic characterstic of noscapine has ushered in the clinical development of the non narcotic therapeutic as as and anti cancer agent. It has shown potential in phase I/H of clinicial studies. Noscapine has been found in studies to reduce cell growth in a variety of cancer cell, incuding drug resistant types, while having no effect on healthy cells. Compounds that block microtubers activate the mitotic phase control station and stop the cell cycle, causing the tubulin polymer to polymerize more than ususal. Noscapine and its analogues have been demonstrated in order to inhibit skin, ovarian, blood, breast and giloblastoma tumours wihout inducing dose-dependent toxicity in the heart, liver, kidney, bone marrow, spleen and small intestine tissues. Despite the significant potential of noscapine and its analougues there is still a need of mechanistic and preclinical pharmacological studies are required to achieve maximum efficacy of the drug.

Contents

1. Introduction 2. Review of literature 3. Aim and objective 4. Synthesis and characterization of novel 1, 3-benzodioxole tagged noscapine based ionic liquids with in silico and in vitro cytotoxicity analysis on HeLa cells 5. Mechanistic interaction of triflate based noscapine ionic liquid with BSA: spectroscopic and chemoinformatics approaches 6. Unraveling the interaction of an opium poppy alkaloid noscapine ionic liquid with human haemoglobin: biophysical and computational studies 7. Evaluation of interaction between noscapine-based ionic liquid and calf thymus DNA: spectrophotometric and computational methods. Summary. Research publication.

43. SHAH (Chandan)

Synthesis of Functionalized 2-(Alkynyl)benzonitriles, 1,2,3,5-Tetrahydroimidazo[1,2-a]pyridines, Quinolines, Isoquinolines and 2H-Pyran-2-ones from Ketene Dithioacetal.

Supervisor: Prof. Ramendra Pratap

Th 26593

Abstract

The thesis includes design, synthesis, structural elucidation, and mechanistic investigation of 2-(alkynyl)benzonitriles, 1,2,3,5-tetrahydroimidazo[1,2-a]pyridines, isoquinolines, quinolines, and 2H-Pyran-2-ones. Further, these primary molecules are used for further modification. These compounds were synthesized using ketenedithioacetals as precursors. In addition, molecular docking studies of the synthesized compounds were also conducted. The thesis content is divided into four chapters. Chapter 1: Synthesis of functionalized 2-(alkynyl)benzonitriles and their molecular

docking study as aromatase receptor. Chapter 2: Domino synthesis of functionalized 1,2,3,5-tetrahydroimidazo[1,2-a]pyridines from ketene dithioacetals and molecular docking with DNA gyrase. Chapter 3: I2/DMSO-promoted synthesis of multifunctional quinolines/isoquinolines and docking study for anticancer activity. Chapter 4: Design and synthesis of 6-aryl-4-sec.amino-2-oxo-2H-pyran-3-carbonitriles derivatives as PPAR-γ agonists. Chapter 1: In this chapter, we are reporting the synthesis of various functionalized terminal and internal 2-(alkynyl)benzonitriles by using 6-aryl-4-sec.amino-2-oxo-2H-pyran-3-carbonitriles and 4-(trimethylsilyl)but-3-yn-2-one/4-phenylbut-3-yn-2-one as precursors. We have also investigated the mechanistic approach for the synthesis of functionalized 2-(alkynyl)benzonitriles. Chapter 2: In this chapter, we have developed a methodology to synthesise 1,2,3,5-tetrahydroimidazo[1,2-a]pyridines using 1,6-Michael acceptor ketene dithioacetals under mild conditions. The structure of all the synthesized compounds (1,2,3,5-tetrahydroimidazo[1,2-a]pyridines) was confirmed by the 1H NMR, 13C NMR and HRMS. The structure of one of the compound was confirmed by the single crystal X-ray Chapter 3: In this chapter, we reported iodine and DMSO-promoted synthesis of multifunctional quinolines and isoquinolines using 6-aryl-4-sec.amino-2-oxo-2H-pyran-3-carbonitriles and 1-Boc-4-piperidone/1-Boc-3-piperidone as precursors. The reaction proceeded efficiently, and the desired quinolines/isoquinolines were achieved in good yields. The generality of the protocol was tested by using various functionalized 2-pyranones with 1-Boc-4-piperidone. Chapter 4: In this chapter, we present a 6-aryl-4-sec. amino-2-oxo-2H-pyran-3-carbonitriles derivative as a potential substitute for the 2,4-thiazolidinedione head group that exhibits a potent PPAR-transactivation response.

Contents

1. Synthesis of functionalized 2-(alkynyl)benzonitriles and their molecular docking study as aromatase receptor 2. Domino synthesis of functionalized 1,2,3,5- tetrahydroimidazo[1,2-a]pyridines from ketene dithioacetals and molecular docking with DNA gyrase 3. I_2/DMSO-promoted synthesis of multifunctional quinolines/isoquinolines and docking study for anticancer activity 4. Design and synthesis of 6-aryl-4-*sec.*amino-2-oxo-2*H*-pyran-3-carbonitriles derivatives as PPAR-γ agonists. List of publications.

44. SHARMA (Himshikha)

Synthesis and Characterization of Novel Phenothiazine, Azaphenothiazine and Benzimidazole Derivatives and Their Applications.

Supervisor: Prof. M.D. Milton

Th 27094

Abstract

The describes design, synthesis and characterization of three classes of heterocyclic compounds, namely, phenothiazine, azaphenothiazine and benzimidazole. Novel phenotiaziine compounds were explores for their potential applications like volatile acid/pH sensors, solvent sensors, and temperature sensors. Azaphenothiazine and benzimidazole derivatives were evaluated for biological activities. Benzimidazole derivatives were also explored as metal ion sensors. The present thesis is divided into six chapters. The brief description of the work presented in the thesis is as follows: Chapter 1 deals with the recent literature review on phenothiazine, azaphenothiazine and benzimidazole derivatives and their applications as fluorescent sensors/probes and biologically active molecules. This chapter also discusses the goals of the research work embodied in the thesis. Chapter 2A describes the synthesis of phenothiazine-*5*-oxide derivatives using Suzuki cross coupling reaction. All compounds were characterized by 1H NMR, 13C NMR, HRMS and IR spectroscopy. Two of the compounds were also characterized by single crystal X-ray diffraction (XRD) analysis. A positive solvatochromism was observed with large Stokes shifts. These fluorescent solids showed “on-off-on” response toward TFA (trifuoroacetic acid) vapors, which was reversed in the presence of TEA (triethylamine) vapors. A similar response was also observed in solution. NMR and DFT studies were conducted to explore the interactions between phenothiazine-*5*-oxide dialdehydes and TFA. Filter paper strips for TFA sensing were also fabricated. These compounds are found to exhibit IMPLICATION logic gate operation with TFA and TEA as the inputs. Chapter 2B discusses the synthesis of novel phenothiazine-*5*-oxide bishydrazones using from phenothiazine dialdehydes (prepared in chapter 2A) as the starting material. Bishydrazones were characterized by 1H NMR, 13C NMR, HRMS and IR spectroscopy. The protonation of pyridyl nitrogens leads to remarkable enhancement of fluorescence 2 intensity with red shift under highly acidic conditions due to combined effect of PET-off and strong ICT. Hence, these probes exhibits “turn on” fluorescence sensing towards extreme acidic pH range. Because of two pyridyl units, two pKa values observed in the range of 3.2-4.7. Thus these novel bishydrazone may find applicability in monitoring the pH changes in biological systems. Reversible changes were observed in the respective pH ranges. Moreover, acidochromism studies were also performed with TFA and HCl. Based on reversible acidofluorochromic and pH responses, INHIBIT logic gate was also constructed. Chapter 3 includes design and synthesis of phenothiazine-*5*-oxide derivatives with extended π-conjugation. All the compounds were obtained in good yields 78-87 % and characterized by 1H NMR, 13C NMR, IR and HRMS analysis and three of these compounds were also characterized by single crystal XRD analysis. Single crystal X-ray diffraction studies (XRD) confirmed the disubstitution and trans-configuration along the double bonds. Photophysical studies revealed that on extending π conjugation by introducing vinyl group, the absorbance as well as emission wavelengths are red shifted. Compounds substituted with acrylates showed AIE property while other substituted with styrene showed ACQ property in different fractions of THF/water. Positive solvatochromism was observed for all compounds. Temperature based emission behavior was explored. Additionally, good to excellent thermal stability was indicated by thermogravimetric analysis with the thermal decomposition temperature (Td) in the range of 200-308oC. Chapter 4 describes the synthesis of novel substituted *1*-azaphenothaizine and its *10*-(*2′*-morpholinylethyl) derivatives and investigation of their biological activities. All new compounds were characterized by 1H, 13C NMR, HRMS and IR spectroscopy. Single crystal X-ray diffraction (XRD) analysis also confirmed the structure of one of the compound. These compounds were evaluated for anticancer screening test against various cancer cells such as MCF-7 (breast), MDA-MB-231 (breast), CaCO2, SW48 (Colon), A549 (lung), SW1190 (pancreatic) and HEK293 (non-cancer Kidney) cells. These experiments revealed that *10*-(*2′*-morpholinylethyl) derivatives are more potent than *1*-azaphenothaizine derivatives. And some compounds exhibit better IC50 values against colon cancer cell and breast cancer cell. 3

Chapter 5 includes the synthesis of *N, N'*-disubstituted benzimidazolium salts in excellent yields 93-98%. The synthesized products were characterized by 1H NMR, 13C NMR, IR and HRMS. The structure of one of the benzimidazolium salt was also confirmed by single crystal X-ray analysis. These salts exhibited a selective “turn-off” fluorescence response towards Fe3+ ions in aqueous solution over the other competitive metal ions such as Ag+, Al3+, Ba2+, Ca2+, Co2+, Cr3+, Cu2+, Fe2+, Fe3+, K+, Mg2+, Na+, Ni2+, Pb2+ and Zn2+. Detection limit for all probes with Fe3+ ions were found in micromolar range. Also, these probes have to potential to detect Fe3+ ions in physiological range. Further, Job’s plot displayed the binding stoichiometry of 1:1 molar ratio between probes and Fe3+ ions. Moreover, drug combination analysis has shown that two of benzimidazolium salts could synergise doxorubicin sensitivity in breast cancer cell line (MDA-MB-468, MDA-MB-231 and MCF7) with promising dose reduction potential between doxorubicin and these compounds in breast cancer treatment. Molecular docking studies were also performed to explore the binding affinity between benzimidazolium salt and chk2 protein. Chapter 6 summarizes the important new findings and conclusions of the research work embodied in the thesis.

Contents

1. Introduction 2A. Design, synthesis and characterization of novel phenothiazine-5-oxide aldehydes and their applications as volatile sensors 2B. Design, synthesis and characterization of D-A based phenothiazine-5-oxide bishydrazones and their applications as reversible pH sensors 3. Phenothiazine-5-oxide based derivatives with extended π-conjugation: design, synthesis, characterization photophysical and thermal studies 4. Substitute *I*-azaphenothaizinen and its *10-(2'*morpholinylethyI) derivatives: synthesis, characterization and biological evaluation 5. Syntheis and characterization of novel dicationic benzimidazolium salts and their applications as Fe(III) ions sensing probes in aqueous media and anti-breast cancer agents 6. Summary and conclusion.

45. SHARMA (Neha)
Mutlistage Antimalarial Evaluation, Lead Optimization and Pharmacological Studies of Novel Hydroxyethlamine Analogs and *N*-Substituted Amines Intriguingly Intervene Growth and Transmission of Malaria Parasite.
Supervisor: Dr. Brijesh Rathi
Th 26594

Abstract

Malaria continues to be one of the deadly infectious illnesses that affects the global human population. According to the WHO's 2021 global malaria report, 241 million malaria cases were reported worldwide in 2020. Life cycle of the malaria parasite starts when a female mosquito bites an intermediate host, and releases sporozoite that settles beneath the skin of the mammalian host. Malaria still affects a significant number of people despite notable advancements in the use of chemotherapy. Major problems with the disease are emergence of resistance for the frontline treatments and unavailability of effective vaccines. The majority of antimalarial medications target blood stage malarial infection and are either ineffective or less

effective against other life stages of the parasite. As the parasite load remains very less in liver stage then this stage could be a prime target for the treatment. Being asymptomatic in nature and also unavailability of dinical models, screening against liver stage is very difficult. Also, no effective drug treatment is available for the transmission stage of parasite rather toxicity is shown by few available antimalarials. According to World health organization, there is an immense need for malaria treatments that target all the life stages of the parasite especially drug molecules capable to kill the parasites of liver stage, gametocyte stage and transmission blocking stages as these stages are essential for preventing disease epidemics and protecting vulnerable populations due to increased asexual antimalarial drug resistance. As WHO has already stopped the use of artemisinin as monotherapy rather it can be used in combination with other antimalarial. So we need to develop new drug molecules that can be used either alone or in combination with artemisinin. Hydroxyethylamine (HEA) pharmacophore have been thoroughly investigated as potent multistage antimalarial drug candidate. In recent years, HEA pharmacophore combined with substituted N-substituted amines was successively examined for multistage antiplasmodial activity that accompanied to a few potent molecules with minimal toxicity.

Contents

1. Introduction: malaria disease, life stages of the parasite, limitations of current therapeutics, and multistage antimalarial drug discovery avenues 2. Design, synthesis and biological evaluation of novel antiplasmodial compounds leverged with high multistage poteny against plasmodium *falciparum*: in *vitro* and in *vivio* evalutaions and pharmacokinetic studies 3. Identification of multistage antimalarial compounds perturbate plasmodium falciparum Ca^{2+} homeostasis by targeting a uniqe ion channel 4. Enhanced multistage antiplasmodial activity of a preclinical candidate against chloroquine resistant malaria 5. Solvent-free mechanochemical supported clean synthesis of N-substituted amines and their antimalarial evaluation. Research publications.

46. SHREYA

Strategies of making defective anatase, cation-modified Co_2 TiO_4,Zn_2MnO_4 systems and their functions.

Supervisor: Prof. Rajamani Nagarajan

Th 27095

Abstract

The work presented in this thesis is based on the various strategies adopted to make TiO2, Ti- and Mn- containing spinels. In the case of TiO2, defective anatase polymorph from a single source precursor of varying color and properties is generated by differing reaction conditions, solvent media, and titanium sources. Cobalt titanates in inverse spinel structural arrangement have been synthesized by a facile co-precipitation method. Efforts towards the structure-property relationship in these systems have been attempted. The relation between structure, cation valences, and magnetic properties has also been probed in spinel systems. Wherever it is deemed required, some of these systems have been applied in catalysis, photocatalysis, and adsorption processes.

Contents

1. Introduction 2. Description of fundamentals of characterization technniques employed in the present study 3. One precursor, many colors: case study of defective anatase 4. Magnetic properties of titanium-containing inverse spinels 5. Synthesis exploration and magnetic property evaluation of zinc-rich spinels 6. Conclusion and future directions. List of publications workshops and conferences attended.

47. SINGH (Amit)
Synthesis of Nano-Formulations for Gene and Drug Delivery Applications.
Supervisor: Prof. Mahima Kaushik
Th 26595

Abstract

Nanotechnology is a field of science and technology that deals with the manipulation and control of matter on the nanoscale, typically ranging from 1 to 100 nanometers. At this size range, materials exhibit unique properties and behaviors that differ from their bulk counterparts. Nanomaterials, which are the building blocks of nanotechnology, possess distinct physical, chemical, mechanical, and electrical properties due to their high surface-to-volume ratio and quantum effects. One significant property of nanomaterials is their enhanced surface reactivity. With a larger surface area available for interaction, nanomaterials can exhibit increased catalytic activity, making them valuable in various industrial applications such as energy production and pollution remediation. Additionally, their unique electronic properties make nanomaterials highly desirable for electronic devices. Nanoparticles can be designed to have specific surface properties that allow them to target specific cells or tissues in the body, which can be beneficial for drug delivery applications. Additionally, the small size of nanoparticles allow them to cross biological barriers more easily, which can improve the delivery of drugs to their target sites. The interaction of DNA and proteins with nanoparticles holds great potential for drug delivery applications. Nanoparticles can serve as carriers or vehicles to efficiently transport DNA or proteins to specific target sites in the body and overcome barriers such as enzymatic degradation and poor cellular uptake. Polymeric nanoparticles have emerged as promising carriers for drug delivery due to their versatility, tunable properties, and ability to encapsulate a wide range of drugs. These nanoparticles are typically composed of biocompatible and biodegradable polymers, offering advantages such as controlled release, protection of drugs, improved bioavailability, and targeted delivery. One of the key advantages of polymeric nanoparticles is their ability to encapsulate both hydrophilic and hydrophobic drugs.

Contents

1. Introduction & review of literature 2. Materials and methods 3. Green synthesis and characterization of Zinc oxide nanoparticles from Azadirachta Indica (Neem) leaf extract and their interaction with calfthymus DNA 4.

Influence of green synthesized Zinc Oxide nanoparticles on molecular interaction and comparative binding of Azure dye with chymotrypsin 5. Systemic co-delivery of mitoxantrone loaded chitosan coated PLGA nanoparticles to improve the chemotherapy against human non-small cell lung cancer 6. Targeted Nanotherapy by vinblastine loaded chitosan coated PLA nanoparticles to improve the chemotherapy against hepatocellular carcinoma Chapter 7 Conclusion. List of publications. Details of conferences.

48. SINGH (Devneder)
Development of Schiff Base-Based Chemosensors For The Detection of Selected Analytes.
Supervisor: Prof. Rajeev Gupta
Th 27096

Abstract

The present thesis is divided into six chapters. Chapter 1: Introduction: Selected Examples of Schiff Base-based Chemosensors for the Detection of Selected Analytes The aim of this chapter is to provide a brief overview of the selected Schiff base-based chemosensors for the detection of various analytes ranging from metal ions to anions to amino acids. Out of various Schiff base-based chemosensors, coumarin-based chemosensors have been thoroughly investigated. Coumarin is a well-known organic chromophore that has been 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. chapter 2 has illustrated the synthesis of two related chemosensors, L1 and L2, containing appended naphthalimide ring(s) as the fluorophore(s). Both chemosensors selectively detected Ni2+ and Zn2+ ions out of assorted metal ions. The coordination of Ni2+ and Zn2+ ions to the chemosensors resulted in prominent changes in their emission and absorption spectra. In chapter 3, a selective, sensitive, and reversible coumarin-benzothiazole-based chemosensor L3 was synthesized via a simple condensation reaction. Chemosensor L3 was utilized for the fluorescent “turn-on” detection of Mg2+ and Zn2+ ions. Emission and absorption spectral titrations allowed the calculation of detection limits and binding constants. Chemosensor L3 showed impressive detection limits and high binding constants for both Mg2+ and Zn2+ ions. The binding studies supported a 1:1 stoichiometry of the chemosensor with the Mg2+ and Zn2+ ions which was further supported by the DFT studies. In chapter 4, two pyrene-linked-coumarin-based chemosensors L4 and L5 were synthesized. The two chemosensors differed by a methylene spacer that connected the coumarin and pyrene rings through an imine group. Both chemosensors L4 and L5 were utilized for the detection of copper and zinc ions, respectively. The inclusion of the methylene spacer dramatically changed the detection profiles of the two chemosensors. chapter 5 presents two Schiff base-based chemosensors **L6** and **L7** offering extended conjugated groups for the primary detection of Cu2+ ion and the secondary detection of citrate ion. In both chemosensors, imine and hydroxyl functional groups were responsible for the selective detection of Cu2+ ion. Both chemosensors formed a 1:1 stoichiometric complex with a Cu2+ ion. DFT studies and HOMO-LUMO calculations further established a 1:1 stoichiometry. The solution-generated [**L6**/**L7**-Cu] adducts illustrated a selective secondary detection of the citrate ion over assorted anions via extrusion of the Cu2+ ion. Both **L6** and **L7** displayed

high emission which was quenched by the Cu2+ ion and then restored by the addition of citrate ion, i.e., an "on-off-on" type system. Such a reversibility also allowed the construction of the molecular logic gates. In chapter 6 presents a coumarin-anthracene-based chemosensor **L8** for the selective detection of Arginine (Arg) via a chemodosimetric approach. Significant changes in both emission and absorption spectra of chemosensor **L8** were observed after the addition of Arg. Chemosensor **L8** displayed an impressive detection limit of 0.46 μM for Arg. Arg assisted dosimetry of chemosensor **L8** was illustrated by a combination of the UV-Vis spectra, NMR spectra, mass spectra, excited-state lifetime studies and quantum yield calculations. The sensing of Arg by chemosensor **L8** was employed in colorimetric detection, paper test-strip detection, PMMA film-based detection and in live cells imaging.

Contents

1. Introduction: selected examples of Schiff base-based chemosensors for the detection of selected analytes 2. 'Turn on' fluorescent detection of nickel and zinc ions by two related phenol-based chemosensors containing nephthalimide ring(s) 3. A coumarin-benzothiazole-based chemosensor for the 'Turn-on' dual-channel discriminative detection of magnesium and zinc ions 4. Methylene spacer mediated detection switch between copper and zinx ions by two coumarin-pyarene-based chemosensors 5. Coumarin-based fluorescent chemosensors offering extended conjugation for the selective detection of copper and citrate ions 6. A coumarin-anthracene-based chemodosimeter for the selective detection of arginine. Summary. List of publications.

49. SINGH (Jagmeet)

Synthesis and Photophysical Properties of Β-Heterocycle-Fused 5, 10, 15, 20- Tetraarylporphyrins.

Supervisor: Prof. Mahendra Nath

Th 26596

Abstract

Porphyrin macrocycles play pivotal roles in diverse biological processes including oxygen transport and photosynthesis. In addition, various periphery modified porphyrinoids with extended π-systems have shown a wide range of material and medicinal applications. By considering these facts, the present research work is focused to design convenient and efficient synthetic strategies for the construction of novel β-heterocycle-fused porphyrins through a peripheral functionalization of easily accessible meso-tetraarylporphyrins and study their photophysical characteristics. The work presented in the thesis is divided into four chapters. The first chapter presents an overview on the synthesis and photophysical properties of previously reported β-heterocycle-fused 5,10,15,20-tetraarylporphyrins. The second chapter discusses about the synthesis, spectroscopic characterization and optical properties of a new series of β-thiophene-fused porphyrins and β-substituted porphyrinic thiazolidinones. These compounds were prepared by the reaction of 2-formyl-5,10,15,20-tetraarylporphyrins with primary amines and mercaptoacetic acid or thiolactic acid in 1,2-dichloroethane at 80 °C under one-pot operation. The third chapter deals with a CuI-catalysed synthesis and evaluation of photophysical properties of newly designed β-oxazole-fused meso-tetraarylporphyrins. The fourth chapter describes a cascade amination and aza-6π-electrocyclization/aromatization reaction of 2-(N,N-dimethylformamidine)-3-formylporphyrin precursors in the presence of aqueous ammonia to afford novel β-pyrimidine-fused 5,10,15,20-tetraarylporphyrins. After chromatographic purification, the newly prepared β-heterocycle-fused porphyrins have been adequately characterized on the basis of spectral data analysis. On photophysical investigation, these porphyrin molecules have shown interesting optical properties with a modest to significant bathochromic shift in their electronic absorption and emission spectra as compared to the traditional meso-tetraarylporphyrins. Hence, the results included in the thesis are useful for the future designing of diverse π-extended aromatic superstructures as light harvesting materials and photosensitizers in photodynamic therapy applications.

Contents

1. Synthesis and photophysical properties of β-heterocycle-fused 5, 10, 15, 20-tetraarylporphyrins: An overview 2. Synthesis, characterization and photophysical studies of novel βthiophene-fused porphyrins 3. CuI-catalyzed synthesis and evaluation of optical properties of βoxazole-fused 5, 10, 15, 20-tetraarylporphyrins 4. Synthesis, spectroscopic characterization and photophysical properties of β-pyrimidine-fused 5, 10, 15, 20-tetraarylporphyrins. Summary. Publications.

50. SINGLA (Harbansh)
Synthesis and Photophysical Studies of Coumarin Triazole Nucleosides & Chemo-enzymatic Synthesis of Modified Pyrimidine Nucleosides.
Supervisor: Prof. B.K. Singh
Th 26597

Abstract

The work presented in Chapter I entitled "Synthesis and photophysical studies on N1-(Coumarin-4‴-yl)-C4-(2′,3′-dideoxyuridin-3′-yl/3′-deoxythymidin-3′-yl)-oxymethyl-1,2,3-triazoles" describes the synthesis of N1-(coumarin-4‴-yl)-C4-(2′,3′-dideoxyuridin-3′-yl)-oxymethyl-1,2,3-triazoles and N1-(coumarin-4‴-yl)-C4-(3′-deoxythymidin-3′-yl)-oxymethyl-1,2,3-triazoles by Cu(I)-catalyzed Huisgen (3+2) cycloaddition reaction. This chapter reports simple and efficient synthesis of a series of twelve novel coumarin triazolylmethyl nucleosides by Cu(I) catalyzed click methodology. The silyl protected O-alkynylated nucleoside precursors were synthesized from the key substrate for [3+2] cycloaddition reaction, i.e. 2′-deoxyuridine and thymidine. The newly synthesized coumarin-triazolylmethyl nucleoside conjugates were found to show better Stokes Shift values in comparison to coumarin-triazolyl bicyclonucleoside conjugates. The work in chapter II reports a simple and efficient method for the synthesis of base modified coumarin-triazole nucleosides by using Cu(I)-catalyzed click methodology and evaluation of their photophysical studies. It was observed that the Stokes shift values of coumarin-triazolyl bicyclonucleoside were 70-78 nm and coumarin-triazolylmethyl nucleoside conjugates were 82-215 nm. While in the present methodology, the Stokes shift values of synthesized derivatives were found to be in the range of 95-296 nm. The work presented in Chapter III entitled "Chemo-enzymatic Synthesis of Bridged

Homolyxofuranosyl Pyrimidine Nucleosides: Bicyclic AZT Analogues" describes the synthesis of (5′R)-3′-azido-3′-deoxy-2′-O,5′-C-bridged-β-D-homolyxofuranosyl pyrimidine nucleosides by chemoenzymatic approach. Nucleoside monomer of locked nucleic acid, i.e. (5′R)-3′-azido-3′-deoxy-2′-O,5′-C-bridged-β-D-homolyxofuranosyl-thymine was found to be locked into C3′-exo sugar puckering with pseudo rotational phase angle (P = 199.02°), indicating the S-type conformation of the nucleoside. The work presented in Chapter IV entitled "Chemo-enzymatic Synthesis of Bridged Homoarabinofuranosyl Pyrimidine Nucleoside" describes the synthesis of (5′R)-2′-O,5′-C-bridged-β-D-homoarabinofuranosyl pyrimidines by incorporating enzymatic step with an effective overall yield starting from diacetone-D-glucofuranose. Nucleoside monomer of bridged-nucleic acid, i.e. 2′-O,5′-C-bridged-β-D-homoarabinofuranosyl-thymine was found to be locked into C3′-exo sugar puckering with pseudo rotational phase angle (P = 196.11°) indicating the S-type conformation of the nucleoside.

Contents

1. Synthesis and Photophysical Studies of N ^{1} -(Coumarin4'''-yl)-C ^{4} -(2',3'-dideoxyuridine-3'-yl/3'-deoxythymidine3'-yl)-oxymethyl-1,2,3-triazo 2. Synthesis and Photophysical Studies of 5-(N ^{1} ''-(Coumarin4'''-yl)-1'',2'',3''-triazoles-4''-yl)-2',3',5'-tri-O-acetyl/3',5'- di-*O*-acetyl-2'-deoxyuridine 3. Chemoenzymatic Synthesis of Bridged HomolyxofuranosylPyrimidine Nucleosides: Bicyclic AZT Analogues 4. Chemoenzymatic Synthesis of arabino-Configured Bicyclic Nucleosides. Summary. List of Publications. Workshops and Conferences attended.

51. SUMIT KUMAR
Computational Accelerated Development of Potent Scaffolds and Their Biological Assessment Against Sara-Cov-2.
Supervisor: Dr. Poonam
Th 27097

Abstract

A virus belongs to the genus category as per the International Committee on Taxonomy of Viruses (ICTV), which further extended to the upper level such as family, order, class, phylum, kingdom, and realm. Accordingly, the coronavirus (CoV) belongs to the Coronaviridae family and ultimately to the Riboviria realm. CoV is a large group of viruses consisting of a core of genetic material enveloped with a protein spike appearing like a crown, which means "corona" in Latin. It was first discovered in a human in the 1960s and to date, a total of seven strain of the virus is known which can cause diseases in humans. Four (229E, OC43, NL63, and HKU1) out of seven strains are responsible for mild disease, whereas the other three are more serious and can cause fatal diseases in humans. The three deadly strains of coronavirus are; SARSCoV (Severe acute respiratory syndrome coronavirus), MERS (Middle-East respiratory syndrome coronavirus), and SARS-CoV-2, the latter was found in late 2019. It is zoonotic and belongs to a large family of viruses, however, the actual zoonotic origin is yet to be confirmed. In late 2002, a coronavirus named SARS-CoV caused several deaths. Likewise, MERS-CoV was responsible for several deaths in the year 2012. Origin of SARS-CoV and MERS-CoV was reported from bats, and the infection was transmitted to humans from civet cats and dromedary camels, respectively. Now, almost after seven years, a novel coronavirus caused an outbreak of pneumonia in Wuhan, Hubei Province of China in late 2019. A rapid team of researchers from the Shanghai Public Health Clinical Center and School of Public Health jointly evidenced the origin of this coronavirus (novel coronavirus, nCoV) from a seafood market in Wuhan city on 7 January 2020. SARS-CoV-2 has caused a recent pandemic called COVID-19 and a severe health threat around the world. For the second year the COVID-19 pandemic has swept the world and for yet another year intensive research is underway aimed at finding the most suitable and effective therapy for the treatment and prevention of the coronavirus infection and the complications caused by the disease. The development of new drugs to circumvent the spread of the virus is of utmost importance.The faster pace of drug repositioning in the treatment of diseases which often relies on serendipity offers a valuable option, especially in a pandemic situation like COVID-19. It could bridge the gap arising from treatment failure, and the time and cost of future drug developments by identifying suitable candidates for novel therapy. This should run in parallel with targetbased studies. Expedition of the drug discovery timeline is crucial and drug repositioning could be used as one of the methods for developing new anti-SARS-CoV-2 agents.

Contents

1. COVID-19: review on drug repurposing forecasted by computational approaches 2. In-silico studies of FDA-approved and in house library of potent scaffolds for the identification of hit analogs against SARS-CoV2 3. Synthesis, characterization and biological studies of aniline-based novel compounds against SARS-CoV-2 4. Design, synthesis and biological evaluation of piperazine-based functionalized compounds against SARS-CoV-2 5. Hit to lead optimization of biological active compounds effective against SARS-CoV-2. Concluding remarks and future plans.

52. SUSHMA
Exploration of Biogenically Synthesized Semiconductor Nanoparticles and Nanocomposites for Environmental Remediation.
Supervisor: Prof. Priti Malhotra
Th 26598

Abstract

Innovations in the area of semiconductor NPs and NCs offer a plethora of applications In the field of catalysis, sensors, solar cells, optics, and environmental remediation. These NPs and NCs have developed photocatalytic reactions in numerous ways by imiting the energy, amount of substrate, time, and catalyst. The properties of these NPs can be altered by varying the shape, size, and dimensions of the materials. Among the two synthetic approach (top-down and bottom up), the bottom-up approach or self- assembly of molecules, atoms, or clusters is utilized in this thesis for the production of semiconductor nanomaterials of different types. The key objective of this work is to design an efficient, eco-friendly, and economic methodology for the synthesis of various types of semiconductor nanomaterials for numerous photocatalytic/ sonocatalytic applications. We utilized simple, non-toxic, and cost-effective protocols mainly agro-waste extracts for the preparation of these NPs and NCs. The agro-waste (sugarcane bagasse and orange pomace) contains various phytochemicals

which are responsible for the reduction and stabilization of metal ions. In this thesis an environmentally benign route was followed for the synthesis using agro-waste sugarcane bagasse and orange pomace for the following reasons: The easy availability of these agro-wastes near laboratory The recycling of these agro-wastes minimizes the pollution Use of biogenic universal solvent ie, water for the synthesis .The biomolecules present in agro-wastes are responsible for the reduction of metal ions and stabilization of the NPs and NCs. Why Sugarcane bagasse? Cancer is the leading cause of death worldwide and a key impediment to increasing age. According to a recent report, cancer accounts for one in every six deaths. Cancer has a Significant impact on worldwide health**,** and this pathology requires innovative erapies that can minimize or eliminate the side effects currently associated with conventional therapies. Noscapine having various pharmacological uses as anticancer drug has evolved as a potential chemotherapeutic agent. The anti-mitotic characteristic of Noscapine has ushered in the clinical development of the non-narcotic therapeutic as an anti-cancer agent. It has shown potential in phase I/II of clinical studies. Noscapine has been found in studies to reduce cell growth in a variety of cancer cells, including drug-resistant types, while having no effect on healthy cells. Compounds that block microtubules activate the mitotic phase control station and stop the cell cycle, preserving the balance between the tubulin polymer and the monomer which may causing the tubulin polymer to polymerize more than usual. Noscapine and its analogues have been demonstrated in order to inhibit skin, ovarian, blood, breast, and glioblastoma tumours without inducing dose-dependent toxicity in the heart, liver, kidney, bone marrow, spleen, and small intestine tissues. Despite the significant potential of noscapine and its analogues, there is still a need for the development of new noscapine analogues and a large number of mechanistic and preclinical pharmacological studies are required to achieve maximum efficacy of the drug. The pharmacokinetic profile of Noscapine is yet to be investigated, thus we have used a variety of biophysical and in silico methodologies to evaluate its capabilities.

Contents

1. Introduction 2. Experimental techniques 3. Sugarcane bagasse facilitated benign synthesis of Cu_2O nanoparticles and its role in photocatalytic degradation of toxic dyes: a trash to treasure approach 4. Biological extract facilitated Cu_2O/ZnO nanocomposites for detection of silver ions in water for environment remediation 5. Orange peel derived Cu2O/RGO nanocomposite: mesoporous binary system for degradation of doxycycline in water 6. Distinguished performance of biogenically synthesized reduced-grphene-oxide-based mesoporous Au-Cu_2O/RGO ternary nanocomposites for sonocatalytic reduction of nitrophenols in water 7. Conclusion. List of publications and conference attended.

53. TOMAR (Anubha)
To Investigate the Impact of Extra Phase of Co_3O_4 on the Electrochemical Performances of Various Ternary Metal Oxide Anodes for Lithium-Ion Battery Application.
Supervisor: Dr. Alok Kumar Rai
Th 26599

Abstract

The development of high-performance anode materials for next-generation lithium-ion batteries (LIBs) is vital to meet the requirements for large-scale applications ranging from electric vehicles to power grids. Conversion-type transition-metal oxides (TMOs) are found to be attractive anodes for next-generation LIBs. Recently, binary and ternary metal oxides based on the transition metals such as Fe, Mn, Ni, Co, Zn etc., have been actively proposed as a replacement of commercially used graphite anode due to their high theoretical specific capacity (>500 mAhg-1), excellent electrochemical properties, high abundance, low-cost, and environmental friendliness. Since binary TMOs have shown high reversible capacities, however they are suffering from low coulombic efficiencies, unstable SEI-layer formation, and poor capacity retention. Compared to binary TMOs, ternary metal oxides exhibit better electrochemical performances due to the distinctive chemical component, variable oxidation states, abundant active sites and high redox activity. Currently, the spinel cobaltite (ACo2O4) have attracted wide attention in energy storage materials for LIBs applications. However, the LIB application of ACo2O4 as anode is still limited due to its drastic volume changes during charge/discharge and poor long-range cycling performances. To overcome the issues of ACo2O4, we made the strategy in the current thesis work to fabricate a mix phase of nanocomposite of binary (Co3O4) and ternary metal oxides (ACo2O4) by partially substituting toxic Cobalt in Co3O4 using various eco-friendly and cheaper transition metal ions (such as A= Ni, Mn, Zn, Cu) to improve the electrochemical performances of ACo2O4 host anode for LIBs. The synthesis of different nanomaterials were performed using cost-effective facile hydrothermal method and polyol-assisted pyro synthesis method. Thereafter, the obtained materials were systematically characterized followed by electrochemical testing as anode for LIB. The nanocomposite electrode (ACo2O4/Co3O4) exhibits superior performances than pure ternary electrode due to the existence of extra phase of Co3O4 in the sample.

Contents

1. Introduction 2. Synthesis Procedure, Characterization Techniques and Electrochemical measurements 3. Facile hydrothermal synthesis of Co_3O_4 as anode material for lithium-ion batteries 4. Boosting the high-rate performance of lithium-ion battery anode using $MnCo_2O_4/Co_3O_4$ nanocomposite interface 5. Insights in utilizing $NiCo_2O_4$/Co3O_4 nanowires as anode material in lithium-ion batteries 6. Synergistic effect between $ZnCo_2O_4$ and Co_3O_4 induced superior electrochemical performances as anode for lithiumion batteries 6. $CuCo_2O_4$ nanoparticles decorated with binary metal oxide as excellent anode material for lithium-ion batteries. Summary. Future scope. List of publications. List of conferences.

54. TOMAR (Deepak)
Synthesis and Theoretical Studies of Transition Metal Complexes as Sensors and Evaluation of their Bioactivities.
Supervisor: Prof. Aruna Chhikara
Th 26600

Abstract

Metal-based drugs have been intensively explored in the pharmaceutical, biochemistry, agricultural, and clinical industries since the serendipitous discovery of the chemotherapeutic agent *cis*-platin. Because of its flexible bonding properties and diverse pharmacological properties, coordination chemistry has been extensively studied. Metal complexes exhibit a wide range of characteristics such as electrochemical, catalytic, photovoltaic materials, enzyme inhibitory, lipid-lowering properties, photodynamic therapy, and biological properties like antibacterial, antitumor. antifungal, antioxidant, anticonvulsant, anti-inflammatory, anti-viral, antifertility, anti-HIV, anti-proliferative, diuretic activities. Metal complexes demonstrate higher biological activity than their respective ligands. Antibiotic resistance is a serious problem nowadays, thus new drugs with a broad spectrum of action and no or minimal toxicity are needed. Metal complexes have low stability and solubility, making them difficult to introduce into clinical practice. In this present study we have synthesized ligands, their metal complexes and characterized them by the various spectroscopic techniques. All the complexes of the ligands have the ability to interact with the BSA and few ligands showed naked eye colorimetric chemosensor properties. Ligand L1 was synthesized by the condensation of 4-tertbutyl benzohydrazide and furan-2-aldehyde. Four different Co (II), Ni (II), and Cu (II) complexes of ligand LI were synthesized. Octahedral geometry of Co (II) complexes, tetrahedral geometry of Ni (II) complex, square planar geometry of Cu (II) was established by the experimental studies and also hold true with the theoretical studies. Chemical hardness, dipole moment and chemical softness of L1 and its metal complexes were studied by DFT. Antibacterial activities of ligand L1 and its complexes were evaluated by modified agar well diffusion method. Molecular docking results of BSA also showed good correlation with the experimental result. Ligand L2 was synthesized by the condensation of 3,5- dichlorosalicylaldehyde and 4-phenylsemicarbazide. Co (II), Ni (II), Cu (II) and Zn (II) complexes were synthesized in 1:1 molar ratio of metal to ligand. The thermal stability of the complex was studied by TGA method. By using DFT, the geometries of Schiff bases and metal complexes were fully optimized. On the basis of spectral studies, an octahedral geometry has been assigned for Co (II), square planar for Cu (11) *and* tetrahedral for Ni (II) and Zn (II) complexes. The antimicrobial activities were examined against human pathogenic strains. The biological activity of ligand L2 was established by MTT assay. Screening against mouse fibroblast cell line was performed, salt indicates that metal complexes show increase in cytotoxicity in proliferating cell line as compared to the free ligand. We have reported the synthesis of a novel (E)-2,4- dichloro-6-(((5-mercapto-1,3,4-thiadiazol-2-yl)imino)methyl)phenol (L3) and its role as a colorimetric sensor for selective detection of Cu (II)., another novel ligand 3-(2- piperidin-1-*yl*)-2-selenoxoacetyl)-2H-chromen-2-one (L4) and its role as a colorimetric sensor for selective detection of Hg (II).

Contents

1. Introduction 2. Synthesis, spectral characterization, theoretical calculations, antimicrobial activity and BSA binding of Co(II), Ni(II) and Cu(II) novel complexes with schiff base ligand L1 3. Synthesis, spectral characterization, DFT calculations, antibacterial and MTT assay of Co(II), Ni(II), Cu(II) and Zn(II) Complexes with Novel schiff base ligand L2 4. Thiadiazole functionalized salicylaldehyde-schiff base as a highly selective

pH-responsive and chemo-reversible “Turn-Off” fluorescent probe for selective Cu (II) detection up to micromolar concentration in semiaqueous media: logic gate behaviour and molecular docking studies 5. Synthesis and application of 2-selenoxoacetyl coumarin derivative as a colorimetric sensor for selective detection of Hg(II) 6. Summary and conclusion. List of publication.

55. UPADHYAY (Charu)

Novel Fluorinated Compounds Potent Against Malaria Parasite: In Vitro and In Vivo Anti Plasmodial Studies.

Supervisor: Dr. Poonam

Th 27089

Abstract

200 million people globally, primarily in tropical and subtropical areas, are affected by malaria, one of the most fatal and crippling diseases. The deadliest strain of malaria in humans is Plasmodium falciparum (Pf), one of the five Plasmodium species. The first-line treatments for malaria in sub-Saharan nations include quinolines, aphthoquinones, antifolates, 8-aminoquinolines, endoperoxides, and combinations based on artemisinin (ACT). Drug resistance is unavoidable despite ongoing efforts to discover new medications and treat disease. The most effective method of treating malaria, however, is ACT therapy. Recent observations show that ACT resistance has grown as a result of frequent use. Designing novel antimalarial medications that are powerful, efficacious, and preferably active beyond asexual blood-stage action is important given the current situation.

In the field of medicinal chemistry, the incorporation of fluorine into ligands has long been recognised as a promising technique. Fluorine is frequently used in pharmaceuticals due to its favourable properties, including its small size, metabolic stability, high lipophilicity, and most distinctively its tendency to prolong the half-life of medications. Molecule fluorination has shed lighter on the compounds' metabolic studies. Fluorine was first used in drug creation in 1955, and its pharmacological effects are still being seen today. Thirteen fluorine-containing medications received US FDA approval for commercial use in the year 2020. Building new potent antimalarial drugs with better activity and pharmacokinetic features may require integrating fluorine chemistry into the drug design process. Fluorinated substituents like -CF3, -SCF3, -SFs, and -OCF3 alter the compounds' acidity or basicity, which affects how well they perform biologically. Chemical compounds with promise antimalarial action (both in vitro and in vivo) may be selectively fluorinated to boost their lipophilicity, maintain their acidity, and prevent their ability to oxidise, therefore avoiding unfavourable metabolic pathways and enhancing antimalarial activity. We firmly believe that the rational and conventional design of fluorinated compounds could be a successful method for creating novel antimalarial medications with increased activity. Overall, the steadily growing trend of fluorine chemistry expertise in academia and the pharmaceutical industry will undoubtedly be helpful for the development of novel therapeutic compounds in the future that have greater effectiveness against the malaria parasite.

Contents

1. Review on the importance of fluorinated scaffolds for the discovery of potent antimalarial compounds 2. Sythesis characterization and computational studies of derivatives of ethanolamine containing functionalized heterocyclic compounds and their antiplasmodial evaluation against numan malaria paratise plasmodium falciparum 3. Synthsi, characterization and in-silico studies of new analogues of piperzine containing fluorinated heterocyclic compunds and their in vitro and in vivo studies against multiple stages of malaria parasite 4. Design and development of sulphonamide and sulfonyI based fluotinated heterocyclic compounds and their biological assessment.

56. UPADHYAY (Ravindra Kumar)
Design, Synthesis and Pharmacological Evaluation of Indolines and Benzothiazole Scaffolds.
Supervisor: Prof. Rakesh Kumar
Th 26601

Abstract

This thesis is divided into four chapters. Chapter I briefly describes the literature survey about the recent advances in the field of biological evaluation of heterocyclic scaffolds such as benzothiazole, isatin, pyran and 1,2,3- zole derivatives. Benzothiazole are a significant class of N-heterocycles that constitute portant benzene fused thiazole bicyclic ring scaffolds, with beneficial biological and pharmacological properties. The fascinating finding from studies on the structure-activity relationship is that altering the structure of a substituent group at the C-2 position frequently causes that group's bioactivity to change. Among those 2-amino benzothiazole derivatives with N-substitutions have already attracted considerable attention due to their potential bioactivities. High antiviral activity is shown by 2-aminobenzothiazoles, which is particularly significant during current global COVID-19 epidemic. They also possess, anti-inflammatory, antimicrobial, antioxidant, analgesic, antidepressant, anticonvulsant, anti-diabetic, anticancer, and antituberculosis activity. Chapter II deals with the synthesis of benzothiazole appended bis-triazoles based structural isomers with promising antifungal activity against Rhizoctonia solani. The agricultural industry is scrambling at a great pace to meet the requirements of food for the exponentially growing world population. One of the major hurdles in fulfilling global food security is debilitating plant diseases. These diseases are responsible for both low yield and low quality of food grains leading to a substantial economic loss for the country. Phytopathogenic fungi, a group of many plant pathogens, cause a wide variety of crop diseases. According to the statistics of the World Harvest of Food and Agriculture Organization of the UN (2009-2010), pathogenic fungi particularly, Rhizoctonia solani Kuhn fungus. globally affect five major crops namely, rice, wheat, maize, potatoes, and soybean. Two novel series (5a-f, 6 and 7a-f, 8) of benzothiazole appended bis-triazole derivative-based fungicides that are structural isomers of each other were synthesized using click chemistry and were evaluated for their antifungal activity. The synthetic procedure reported here is highly reliable, simple, and quite reproducible. Chapter III deals with the design, synthesis and biological evaluation of newer triazole based spirooxindoles as potent anti breast cancer agent. It is commonly recognized that cancer is a complex

multifactorial disease and, therefore, cannot be treated with single-drug therapy hence; the development of novel, efficient, and less toxic anti-breast cancer agents remain an important and challenging goal of medicinal chemists in the present era. Accordingly, new agents combining diverse pharmacophores in a single hybrid molecule might represent a goal for the treatment of cancer and indeed a big effort has been put into the identification of anticancer multitargeted hybrid agents. This could be achieved by modifying the most popular pharmacophores as multi-targeting agents. the hybrid molecules obtained by the bio-conjugation of a broad spectrum of heterocyclic derivatives for multi-drug therapy. Spiro compounds have long been preferred in organic synthesis due to a variety of significant biological actions, including anti-tumor, anti- inflammatory, antimicrobial, antitubercular and acetyl cholinesterase-inhibitory properties. Chapter IV deals with Design, Synthesis, and Molecular Docking Studies of Indoline Hybrids. Indoline scaffold is present in many natural products and biologically active compounds suct as antihypertensive drug and angiotensin-converting enzyme inhibitor. The Indoline structure resembles betanidin that is a member of the betalain natural product, the pharmacologica activity of indole-2, 3-dione derivatives is intriguing, and they are widely used as antifungal antiviral, anticonvulsant, antibacterial and anti-Alzheimer. Due to the synthetic versatility of isatin, it is used as a precursor for drug synthesis and it can also be used for the synthesis of various heterocyclic compounds such as indoles and pyrrolidine. Similarly, Spirocyclic core- containing compounds containing indoline scaffold have significant pharmacological effects The establishment of spiroheterocyclic compounds require specific design strategies as its synthesis has always been challenging for the organic chemists. Polycyclic rings fused at a central carbon atom are termed as spirocyclic compounds.

Contents

1. Introduction 2. Synthesis of Benzothiazole appended bis-triazoles based structural isomers with promising antifungal activity against rhizoctonia solani 3. Design, synthesis and biological evaluation of newer triazole based spirooxindoles as potent anti breast cancer agent 4. Design, synthesis and molecular docking studies of newer indoline hybrids. Summary.

57. VERMA (Abhishek)

Synthesis and Characterization of Rhodamine Based Chemosensor and Antimalarial *N*-Heterocyclic Scaffolds.

Supervisor: Prof. Rakesh Kumar

Th 27099

Abstract

This thesis is divided into four chapters. A brief account of each chapter is given below. Chapter 1 briefly describes the literature survey about the recent advancement in the field of chemosensors designed for probing metal ions with a focus on rhodamine based derivatives. The recognition and sensing of environmentally and biologically important species has emerged as a significant goal in the field of chemical sensors in recent years. Extensive efforts have also been carried out for designing of chemosensors for the detection of metal ions in various biological systems. Various colorimetric and fluorescent based methods are quite convenient, economic, specific, and fast, offer high selectivity and sensitivity and does not require any sample pre-treatment thereby making it a promising and desirable technique. Rhodamine dyes are extensively employed as fluorescent probes owing to their photostability, high fluorescence quantum yield, large molar extinction coefficient, low wavelength emission and visible light extinction. The mechanism of rhodamine based chemosensors is due to the reversible ring opening of spirolactam (non-fluorescent) to the amide form (fluorescent) that leads to changes in color. Chapter 2 deals with synthesis of glycerol-triazole conjugated rhodamine based derivatives for colorimetric and fluorimetric sensing of Cu2+ ions, This chapter describes the design and synthesis of glycerol-triazole tethered rhodamine based colorimetric and fluorimetric sensor the selective recognition of Cu^{2+} ion. The sensor allows naked eye detection of Cu^{2+} ions with a fast response (< 1 min). Among the various metal ions tested, the sensor shows selective binding with Cu^{2+} ions only through turn-on fluorescence mechanism. The sensor shows 1:2 binding stoichiometry with binding constant, $K_a = 1.1 \times 10^6$ M^2 as revealed by Job's plot & Benesi-Hildebrand plot (B-H plot), respectively. The detection limit of the sensor with Cu2+ ions is found to be 3.3 µM. Further, the experimental results are also validated using density functional theoretical (DFT) study. Chapter 3 describes the synthesis of triazole conjugated benzimidazole derivatives which are screened for their antiplasmodial activity against Plasmodium falciparum. Malaria is caused by the Plasmodium parasites. These parasites are dispersed to people by the biting of infected female Anopheles mosquitoes, called "malaria vectors". Malaria is caused in human beings by five parasite species out of which two species, Plasmodium falciparum and Plasmodium vivax, result in the alarming threat. Plasmodium vivax is the most prominent parasite in the WHO's America Region, resulting in 75% of total malaria cases in this region. Chapter 4 deals with synthesis of a series of compounds containing hydroxyethylamine-piperazine analogs. Hydroxyethylamine (HEA) based molecules have been explored as strong antimalarial agents and also identified as inhibitors of malarial aspartic proteases. HEA moiety is a stabilized peptidomimetic blocker of aspartic proteases, plasmepsins. HEA, the B- alcohol is an important structural constituent, simulating a tetrahedral intermediate during the breakage of peptide bonds of aspartic proteases; hence, it plays an important role in the antimalarial action.

Contents

1. Recent developments in the field of chemosensors designed for probing metal ions with a focus on rhodamine based derivatives 2. Glycerol-triazole conjugated rhodamine as colorimetric and flurometric sensor for Cu^{2+} 3. Triazole conjugated benzimidazole derivatives: synthesis and evaluation of their antiplasmodial activity against *plasmodium falciparum* 4. Synthesis and characterization of novel hydroxyethylamine-piperazine analogues as potent antimalarial agents. Summary.

58. VERMA (Diksha)
Synthesis of Non-Ionic Amphiphillic Architectures & Fused Dipeptidomimetics for Biomedical Applications.
Supervisor: Prof. Sunil K. Sharma
Th 27100

Abstract

The thesis is divided into four chapters. *Chapter I*: Synthesis of *D*-Glucitol based Gemini Amphiphilic Nano-transporters. In the recent years, ecarbohydrate-based transport systems, also known as glycotargets have received much attention as drug delivery systems. *Chapter II*: Evaluation of Transport Potential of Alkylated and Fluoroalkylated Amphiphilic Hybrid Nano-architectures. The amphiphiles studied so for generally consist of long alkyl chains as lipophilic segments, a new trend is emerging in recent years where fluoroalkyl/perfluoroalkyl chains have been incoprporated in place of alkyl chains, which results in entirely different structures of enhanced stability. *Chapter III*: Synthesis of Non-ionic Amphiphile as Nanocarriers for Biomedical Applications. With the advancement of research in the pharmaceutical sectors and improved understanding has led us to conclude that the conventional drug delivery systems no longer fulfil the requirements to deliver newer type of drug candidates explored in recent years. *Chapter IV*: Synthesis and Biological Evaluation of Fused Dipeptidomimetics. Peptides are the bioactive compounds that play a crucial role in cellular regulation. They generally exhibit high specificity and target affinity, making them appealing scaffolds for designing the newer therapeutics.

Contents

1. Synthesis of D-glucitol based Gemini amphiphillic nano transporters 2. Evaluation of transport potential of alkylated and fluoroalkylated amphiphillic hybrid nano-architectures 3. Synthesis of non-ionic amphiphile as nanocarriers for biomedical applications 4. Synthesis and biological evaluation of fused dipeptidomimetics. Summary.

59. YADAV (Niketa)
Influence of Biocompatible Deep Eutectic Solvents on Protein Structure and Stability.
Supervisor: Prof. P. Venkatesu
<u>Th 26602</u>

Abstract

Proteins are biomacromolecules that functions vital biochemical processes in living beings. Each of them is constituted with unique number and series of amino acid residues. The three dimensional structure of a protein is determined by the amino acids sequence. The structure of protein is stabilized via various interactions including hydrogen bonding, hydrophobic, Van der Waals and electrostatic interactions. The folding of protein is a spontaneous and complex process as it adopts various conformations. The unique structural feathers of proteins are responsible for its function in different biological processes. Additionally, they offer numerous applications in diverse fields of pharmaceutical, cosmetics, textile and bio-industries. The protein behaviour relies on its surrounding medium and its stability is highly sensitive to its interactions with surrounding environment. For a protein to impart its functional characteristics, the maintenance of its native conformation becomes an essential requirement. However, their full scale utilization is restricted due to their inability to sustain their structure against stresses like heat, chemicals and pH which ultimately results in loss of its functionality. Further, any misfolding or unfolding of proteins can result in its aggregation which can be closely associated with lifethreatening ailments like Alzheimer's and Parkinson's disease. Therefore, it is highly significant to understand the protein folding/unfolding mechanism. This would lead to development of new drugs to obviate aggregation and unfolding of proteins. There has been extensive research which suggests methods like protein immobilization, engineering and addition of co-solvents for enhancing the stability and functionality. In this context, deep eutectic solvents (DESS) have emerged as green and designer solvents for protein folding and stabilization. A growing number of reports acknowledge DESS as new generation solvents to address the limitations of conventional solvents towards protein studies. Despite this, DESS are poorly understood at molecular level particularly for bio-based applications and the fundamental aspect of protein stability. Also, there is a dearth of knowledge on counteraction ability of DESs against denatured proteins. Further, there is very limited understanding on the enzyme microstructure in such systems indicating the biomolecular applications. These neoteric solvents have prompted exclusive opportunities in studies dealing with protein stability, increasing the shelf life, improvising enzymatic activity, enhanced thermal stabilization and sustainable bimolecular extraction processes, it becomes obvious to scrutinize the interactions taking place between DESs and proteins/enzymes. Thus, this thesis puts an effort to divulge into the mechanistic interplay between-protein stability in DESs. Also, the counteraction ability of DESS has been assessed.

Contents

1. Introduction and review of literature 2.Material and experiemental techniques 3. Expanding the potential role of deep eutectic sovents towards facilitating the structural and thermal stability of α-chymotrypsin 4. Multifunctional solvothermal carbon derived from alginate using ‘water in deep eutectic solvent; system for enhancing enzyme activity 5. The attenuating ability of deep eutectic solvents towards catboxylated mutliwalled carbo nanotubes induced denatured β-lactoglobulin 6. Assessing the compatiability of choline-based deep eutectic solvents for the structural stability and activity of cellulose 7. Conclusions. Publications.

60. YADAV (Priyanka)

Studies on the Selective Stabilization of a Few Binary and Ternary Metal Oxides Modified With Anion or Cation and Their Applications.

Supervisor: Prof. Rajamani Nagarajan

Th 26603

Abstract

Solid-state chemistry is mainly concerned with developing new synthesis methods, identifying and characterizing materials, describing their structure, and tuning materials with desired and controllable properties. Oxides have been proven to be materials of great interest for various applications based on their stability, ease of synthesis, and handling. Among the various classes of functional materials, metal oxides play a significant role by exhibiting varying physical properties such as conductivity, as conductivity, ranging from superconductivity and metallic down to semiconductors and insulators. Metal oxides show interesting structural, electronic, optical, magnetic, catalytic, and electrochemical properties. These properties can be enhanced by modifying metal oxides with substitution, heterogeneous coupling, polymorphic transitions, tuning size, and varying dimensions.

Specifically, anionic and cationic doping in metal oxides is an efficient strategy to tailor and improve the properties, as mentioned earlier. The structural diversity accompanied by the physical properties and application of oxides is enormous, and researchers consistently contribute to this area by synthesizing new oxides with interesting structures and properties. The present thesis describes the studies on stabilization of the binary and ternary metal oxides modified with anion, cation, and selected applications.

Contents

1. Introduction 2. Graphitic carbon nitride (g-C3N) modified transition metal oxides (M_0O_2,WO_3,TiO_2 and Cr_2O_3) 3. Ordered $LiGa_5O_8$ loaded redox capable $Cu^{2+,}C^{r3}$+-ions:optical, magnetic and catalytic properties 4. Work on lead and sodium-modified praseodymia 5. Rare earth altered bismuth oxide. Conclusion and future directions. List of publications.

61. YADAV (Samanta)
Ruthenium Complexes of Amide-Based Ligands: Synthesis, Characterization and their Catalytic Applications.
Supervisor: Prof. Rajeev Gupta
Th 27101

Abstract

This thesis includes five chapters. Chapter 1 presents an overview of the selected examples of ruthenium complexes reported in literature which are supported with various multidentate ligands and utilize for several fascinating organic transformation. Chapter 2 illustrates the synthesis and characterization of three ruthenium complexes of phosphine amide based ligands and their employment as the homogeneous catalysts for the transfer hydrogenation of assorted ketones including some biological relevant subtrates by using isopropanol as the solvent ketnos including some biologically relevants subtrates by using isopropanol as the solvent as well as hydrogen source. In chapter 3, two sets of ruthenium complexes the [Ru-CI] complexes and their [Ru-H] analogue were synthesized by using heterocyclic-amide based ligands rendering appended phosphine groups. Chpapter 4 presents the synthesis and characterization of a series of ruthenium complexes of coumarin-amide based ligands coordinating to a metal ion in bidentate as well as tridentate manner. Chapter 5 discuss a new class of ruthenium hydride complexes supported with pyridine-amide-based ligands containing appended ester and/or acid grpups.

Contents

1. Selected literature examples of ruthenium complexes supported with multidentate ligands and their catalytic applications 2. Ruthenium complexes of phosphine-amide ligands as efficient catalysts for transfer hydrogenation reactions 3. Hydration of nitriles catalyzed by ruthenium complexes: role of dihydrogen bonding interactions in promoting base free catalysis 4. Base-free transfer hydrogenation of carbonyl compounds catalyzed by ruthenium hydride complexes of coumarin-amide ligands 5. Acceptorless dehydrogenation of amines to nitriles catalyzed by ruthenium hybride complexes of amide-acid/ester ligands. Summary. List of publications.

62. YADAV (Sapna)

Synthesis and Characterization of Nanocomposites and Their Uses as Photocatalyst, Electrochemical Sensor, and Supercapacitor.

Supervisor: Prof. Kalawati Saini

Th 26604

Abstract

Nowadays, nanocomposites have attracted the attention of scientists and researchers due to their applications in physics, chemistry, biology, and materials science. Metal oxide-based nanocomposites are being used as photocatalysts, electrochemical sensors, and supercapacitors. NiO/Co3O4 nanocomposite, NiO/Cr2O3 nanocomposite, ZnO/CuO nanocomposite, and α-Fe2O3/rGO nanocomposites were synthesized successfully using various synthesis techniques. Structural, optical, and morphological analysis of all the synthesized nanomaterials have been done by powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Brunauer-Emmett-Teller (BET), field emission scanning electron microscopy (FESEM), energy-dispersive spectroscopy (EDS), X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FTIR), and UV-visible spectroscopy. Synthesized NiO/Co3O4 nanocomposite exhibited ~89 % photodegradation of methylene blue dye within 360 min under sunlight irradiation. Synthesized NiO/Cr2O3 nanocomposite showed ~93 % photodegradation of methylene blue within 180 min under sunlight exposure and ~88 % of photodegradation of crystal violet dye within 30 min under sunlight irradiation. Synthesized ZnO/CuO nanocomposite exhibited ~99 % photodegradation of methylene blue dye, ~80 % photodegradation of rhodamine B dye and ~67 % photodegradation of methyl orange dye within 180 min under sunlight irradiation. Synthesized α-Fe2O3/rGO nanocomposite showed a high sensitivity and limit of detection of 327.92 μA mM-1 cm-2 and 0.6 mM respectively for electrochemical glucose sensing. Synthesized α-Fe2O3/rGO nanocomposite exhibited a specific capacitance of 310.2 F/g, energy density of 27.54 Wh/kg, and power density of 309.71 W/kg respectively. It can be seen from the above studies that nanocomposites fabricated by different methods are showing different functional properties. Further, more research is required in the area of fabrication and designing of new nanocomposites with enhanced surface area, morphological control, size control, porosity control, and homogeneity of all the homogenous dispersion of all materials in nanocomposites to achieve multifunctional behavior. sites to achieve multifunctional behavior.

Contents

1. Introduction 2. Characterization techniques 3. Synthesis and characterization of NiO/Co_3O_4 nanocomposite for effective sunlight-driven photocatalytic degradation of methylene blue dye 4. Synthesis and characterization of NiO/Cr_2O_3 Nanocomposite for Effective Sunlight-driven Photocatalytic Degradation of Organic Dyes 5. Synthesis and characterization of ZnO/CuO nanocomposite for effective sunlight-driven Photocatalytic degradation of organic dyes 6. Synthesis and characterization of α-Fe_2O_3/rGO nanocomposite for electrochemical glucose sensor and supercapacitor applications 7. Conclusion. List of publications.