# CHAPTER 8

# CHEMISTRY

## Doctoral Theses

01. ANJU
**Development of Metallocomplexes as Molecular Imaging Probes.**
Supervisors : Dr. Firasat Hussain and Dr. Anil Kumar Mishra
Th 25561

*Abstract*
*(Not Verified)*

The thesis entitled “Development of Metallocomplexes as Molecular Imaging Probes” describes the design, synthesis, development, and biological evaluation of metal-complexes as molecular probes for a particular target. The selection of individual précised medicine of requires mapping particular physiological events at the molecular level, and this can be achieved by using highly specific ligand. Targeted probes known as molecular probes, are used to map functional characteristics of a particular target, intracellular communication, and physiological process monitoring. Therefore, the design and development of molecular probes is the primary purpose of the thesis for targeted molecular imaging and validation. The thesis is composed of six chapters. Chapter I: deals with a brief overview of molecular imaging modality and designing parameters of molecule probes. Chapter II: Experimental work, reagents, physicochemical characterization techniques like Density functional theory (DFT), and Computational studies, NMR, ESI-MS, Powder X-ray diffraction, UV-Vis Spectroscopy, fluorescence spectroscopy, MRI are incorporated in this work. Chapter III: This work reports the synthesis and evaluation of 5-HT1A targeted PARACEST MRI contrast agent using (DO3AM) as the bifunctional chelator and 5-HT1A-antagonist MPP as a targeting unit. CEST-related physicochemical parameters were evaluated after loading DO3AM-MPP with paramagnetic MRI active lanthanides: Gadolinium (Gd-DO3AM-MPP). In vivo, MRI studies are performed to evaluate the binding of complex with the 5-HT1A receptor in the brain. Chapter IV: deal with structure-based virtual screening of a hundred plus a library of quinoline drugs with established antiviral, antimalarial, antibiotic, or kinase inhibitor activity to target different proteins of SARS-COV-2. Chapter V: An overview about FAP, design of FAP inhibitor by using docking, synthesis of FAP inhibitor, physiochemical properties evaluation, radiolabeling studies with 99mTc radionuclide have been studied in this chapter. Chapter VI: Brief Explanation about Prostate-Specific Membrane Antigen Inhibitors, synthesis of PSMA targeting Probes, physiochemical properties evaluation, radiolabeling studies have been studied in this chapter.

*Contents*

1. A brief overview about molecular imaging techniques and targeted molecular porbes 2.Physicochemical and biological characterization with their principle and applications 3. 5-$HT_{1A}$ targeting PARCEST agent DO3AM-MPP with potential for receptor imaging: synthesis, physicochemical and MR studies 4. Virtual screening of quinolone derived library for SARS-COV-2 targeting viral entry and replication 5. Design, synthesis and development of $^{99m}$Tc-DTPA-(quinolone)$_2$ as fibroblast

activated protein inhibitor 6. Bivalent approach for targeting prostate specific membrane antigen. Conclusion of the thesis. List of publications.

02. ANKITA
**Physicochemical Studies of Interactions in Solutions Containing Drugs in Misec Aqueous Media.**
Supervisor : Dr. Anil Kumar Nain
Th 25048

*Abstract*
*(Not Verified)*

The work compiled in the thesis entitled "*Physicochemical studies of interactions in solutions containing drugs in mixed aqueous media*"involves the study of solute-solvent and solute-solute interactions within the molecules of aqueous drug and carbohydrate solutions. The thesis work has been divided into eight chapters. Chapter 1 of the thesis is an introductory chapter. It encompasses the scope, significance and objective of the proposed work.Chapter 2 includes the various experimental techniques that have been used for the measurements of density, ultrasonic speed and viscosity of aqueous drug/carbohydrate solutions at different temperatures. The rest of the chapters includesthe volumetric, viscometric and ultrasonic studies of various drugs (isoniazid/ betaine hydrochloride/sodium salicylate/semicarbazide hydrochloride) in aqueous carbohydrate (glucose/sucrose/arabinose/xylose) solutions. These experimental data have been used to calculate various physicochemical properties like apparent and limiting apparent molar volume, apparent and limiting apparent molar compressibility, transfer volume and compressibility from the density and ultrasonic speed measurements while the Falkenhagen Coefficient, *A*, Jones-Dole coefficient, *B* and temperature derivative of *B*-coefficient from the viscosity data. These parameters have been used to discuss the solute-solute and solute-solvent interactions in these systems.

*Contents*

1. Introduction 2. Experimental methods 3.Volumetric, acoustic and viscometric studies of solute-solute and solute-solvent interactions of isoniazid in aqueous-glucose/sucrose solutions at temperatures from 293.15 to 318.15 K 4.Probing solute-solute and solute-solvent interactions of semicarbazide hydrochloride in aqueous-D-glucose/D-sucrose solution at temperatures from 293.15 to 318.15 K 5. Study solvation behaviour and interactions of drug betaine hydrochloride in aqueous-D-xylose/L-arabinose solutions at different temperatures by using volumetric, acoustic and viscometric methods 6. Solute-solute and solute-solvent interactions of drug sodium salicylate in aqueous-glucose/sucrose solutions at temperatures from 293.15 to 318.15 K 7. Study on the interactions of drug isoniazid in aqueous-D-sylose/L-arabinose solutions at different temperatures using volumetric, acoustic and viscometric approaches 8. Molecular interactions of drug semicarbazide hydrochloride in aqueous-D-xylose/L-arabinose solutions at different temperatures: volumetric, acoustic and viscometric study. Conclusion, References and List of publications.

03. ARORA (Gunjan)
**Functionalized Hollow Magnetic Materials as Nanoreactoirs: Fabrication and Catalytic Applications in C-S Cross-Coupling, Halogenation and Multi-Component Reactions.**
Supervisor : Prof. R. K. Sharma
Th 25066

*Abstract*
*(Not Verified)*

The present thesis focuses on design and synthesis of novel magnetically retrievable functional hollow materials as nanoreactors and their catalytic applications in various organic transformations. The work has been divided into six chapters. Chapter I reviews many substantial research contributions with respect to synthetic approaches, functionalization techniques and application aspects of these materials for conducting organic transformations and catalytic degradation of organic pollutants in confined manner. Chapter II provides a general overview of the various techniques used during the entire research work to characterize the obtained composites and products. These techniques include SEM, TEM, FT-IR, XRD, EDX, ICP-MS, XPS, VSM, TGA, BET, GC-MS and NMR. Chapter III describes a novel, facile and straightforward approach to fabricate magnetic carbon nanoreactor consisting of multifunctional double-layered shell, large internal cavity, tailored dimensions and high surface area. The internal cavity of the nanoreactor was filled with copper ions and the catalyst was used to conduct oxidative bromination reaction. Chapter IV illustrates the fabrication of an environmentally benign magnetically recoverable nickel(II)-based nanoreactor *via* a template-free approach. Catalytic performance of the synthesized catalyst is assessed in the confined oxidative coupling of arenethiols with arylhydrazines to form unsymmetrical diaryl sulfides under aerobic conditions. Chapter V elucidates the fabrication and characterization of environmentally benign double-shelled magnetically recoverable cobalt(II)-based hollow composites as nanoreactors. The synthesized composite showed remarkable catalytic efficacy in the synthesis of various thioesters through C-S cross-coupling reaction of thiols with aldehydes. The reactions were carried out in presence of TBHP as an oxidant and water as a green solvent. Chapter VI illustrates the synthesis of functionalized hollow magnetite spheres which were synthesized through gas-bubble assisted Ostwald ripening approach and post-functionalized with sulfamic acid groups. The fabricated material was used as an efficient solid-acid catalyst for one-pot three-component synthesis of medicinally important trisubstituted imidazoles under ultrasonic irradiation.

*Contents*

1. Introduction 2. Theoretical aspects of instrumental techniques used 3. A template-free protocol for the synthesis of copper loaded multifunctional double-shelled $Fe_3O_4$-C nanoreactor for the confined oxidative bromination reaction 4. Fabrication of nickel(II)-loaded magnetically separable nanoreactor scaffold for confined synthesis of unsymmetrical diaryl sulphides in water 5. Magnetically retrievable cobalt-based nanoreactor as an efficient catalyst for the synthesis of thioesters in water 6. Sulfamic acid functionalized hollow magnetically retrievable solid-acid catalyst for the one-pot synthesis of substituted imidazoles under ultrasonic ittadiation. Conclusion, Summary, Spectral data and List of publications.

04. BUNTY KUMAR
**Synthesis of Glycosylated-1,2,3-Triazoles, Glucosylated-1-Azaindolizines, Depsipeptides and Corrosion Studies on Few Chalcones.**
Supervisor : Prof. Prabati Biswas
Th 25074

*Contents*

1. Synthesis, antibacterial and antifungal activities of novel 1-glycosyl-4-aminomethyl-1,2,3-triazoles 2.Synthesis of 2-(β-D-glucopyranosyl)-3-*N*-alkylamino-1-azaindolizines 3.Synthesis of β-*C*-glucoside-based depsipeptides using passerine

reaction 4. Synthesis and corrosion inhibition study on few chalcones. Summary and List of publications.

05. BHUMIKA

**Design of Sustainable Carbon Materials from Biomass/Waste as Energy Efficient Electrode for their Application in Electrochemical Capacitors.**

Supervisor : Prof. Gurmeet Singh

Th 25034

*Abstract*
*(Not Verified)*

The competent cache of electricity induced from greener energy source helps humans getting free from trammel of fossil fuel deficit. Among various ambidextrous materials carbon materials have garner much attention due to their overwhelming properties. Mostly, carbon material reveling remarkable properties are synthesized from fossil fuels by various energy intensive synthetic procedure. Hence, it is an utmost urgency to lower the production cost of these carbon materials while retaining their properties. Carbon synthesized from biomass are excellent material for upcoming energy conversion/storage systems. Chapter 1 and 2 discusses the basics and various characterization technique used to characterize the materials. Chapter 3 focuses on an imperishable approach towards green chemistry by utilizing *Citrus sinensis* peel in energy storage devices. In this, KOH activation at two different temperatures (750 °C & 900 °C) is carried out that result in capacitive oxygen enriched porous carbon. In Chapter 4, we focused on the combined approach by modifying the electrode and electrolyte in order to increase the specific energy of carbon materials. The activated carbon is synthesized from *Citrus limon* peel and electrolyte modification was done by adding HQ to $H_2SO_4$. This work might open a new gateway towards designing high charge storage material through synergism of dopant and redox additive. Chapter 5 substantiates a stratagem for widening potential window in aqueous supercapacitor beyond the water splitting potential (1.23V). A novel asymmetric supercapacitor was fabricated using Sago derived porous activated carbon as negative electrode and $CoSe_2$ nanosheets as positive electrode. Similarly, widening of potential window beyond 1.23 V in aqueous supercapacitor is achieved in chapter 6 through heterojunction design of combining both negative [*Cannabis sativa*] and positive potential material [$VO(OH)_2$] in one electrode. A sustainable and cost-effective precursor for synthesis of negative potential material is utilized that contributes a lot in energy storage system.

*Contents*

1. Introduction 2.Characterization techniques 3. Oxygen rich porous carbon derived from *Citrus sinensis* for high energy density supercapacitor: Biowaste to energy storage approach 4. Synergism between redox active electrolyte and N, P dual doped activated carbon towards high energy density supercapacitor 5. Cobalt selenide sheets and biomass based activated carbon as electrodes for asymmetric supercapacitor 6. Hydrothermal grafting of VO(OH)2 nanotods on hemp stem derived carbon sheet for symmetric 105 V aqueous supercapacitor 7. Conclusion. Appendix and List of publications. Abstract.

06. CHAUDHARY (Neha)

**Physicochemical Studies of Intermolecular Interactions in Multi Component Solvent Systems Containing Polyethylene Glycols and Ionic Liquids.**

Supervisor : Dr. Anil Kumar Nain

Th 25081

*Contents*

07. DANDIA (Anshu)

**Synthesis of Selected Porphyrinoids, Metal Porphyrinoids, Characterization and their Applications in Catalysis and Non-Covalent Interactions.**

Supervisors : Prof. Marilyn Daisy Milton and Prof. S. M. S. Chauhan

Th 25562

*Abstract*

*(Not Verified)*

A brief description of the thesis is divided into five chapters. Chapter 1 deals with the Synthesis of selected tetraarylporphyrins and their regio-specific nitration with nitronium tetrafluoroborate and related nitrating agents. The regiospecific nitration of selected tetraaryl-porphyrins with one equivalent of NO2BF4 to a solution of TPP and TNP in dichloromethane formed an unstable porphyrin-π-cation and NO2-cation-radical. Further, the nitration of TNP with more than 2 equimolar, di-nitration and tri-nitration products were obtained. Chapter 2 deals with the Synthesis of selected manganese triaryl-corroles and their application in the oxidation of selected polycyclic aromatic hydrocarbons. The catalytic amount of manganese(III)-5,10,15-tris(pentafluorophenyl)-corrole and tert-butyl-hydroperoxide in PAH`S (anthracene, benza[a]anthracene, 9-phenylanthracene, naphthalene) have been responsible for the oxidation. Another oxidants like hydrogen peroxide don`t give any adduct by the oxidation of PAH`s. Chapter 3 deals with A one pot reaction of pentafluorobenzaldehyde with thiophene and selenophene in the synthesis of core modified isophlorins and related expanded isophlorinoids. The furan-, thiophene- and selenophene-isophlorins have been synthesized by the reaction of hetero-atoms with BF3.OEt2 and oxidized with FeCl3. Chapter 4 deals with the Synthesis of selected nonplanar porphyrins, their protonation and non-covalent interactions. The peripheral-substituted-porphyrins have been used to prepare the nonplanar-conformations containing suitable model compounds where the steric obstructions presents at the periphery of porphyrin which leads the distorted macrocycles. Firstly, the PAH`s have been nitrated and then convert into PAH containing pyrroles. These pyrroles have been used for the synthesis of non-planar porphyrins. Chapter 5 deals with the Synthesis of perylene-3-aldehyde, coronene-1-aldehyde and their reactions with pyrrole in different reaction conditions. These PAH-containing aldehydes (perylene and coronene) used for the synthesis of PAH containing porphyrins

(perylene and coronene). The reaction of perylene aldehyde with pyrrole doesn't give any porphyrin formation due to the decarbonilation of aldehyde and converts to perylene with pyrrole aldehyde.

*Contents*

1. Synthesis of selected tetraarylporphyrins and their region-specific with nitronium tetrafluoroborates and related nitrating agents. 2. Synthesis of selected manganese triaryl-corroles and their application in the oxidation of selected polycyclic aromatic hydrocarbons 3. A one pot reaction of pentafluorobenzaldehyde with thiophene and selenophene in the synthesis of core modified isophlorins and related expanded isophlorinoids 4. Synthesis of selected nonplanar porphyrins, their protonation and non-covalent interactions 5.Synthesis of perylene-3-aldehyde, coronene-1-aldehyde and their reaction with pyrrole in different reaction conditions.Summary, List of publications.

08. GANDHI (Sona)
**Casein & Ferrite Nanoparticles for Biomedical Applications.**
Supervisor : Dr. Indrajit Roy
Th 25076

*Abstract*
*(Not Verified)*

The ferrite nanoparticles were magnetic in nature; hence, can be used as agents for magnetically guided drug delivery. MFNPs are known to exhibit various biomedical applications, so it is important to understand their biological interactions. We deciphered these interactions using a model protein, bovine serum albumin. The interactions were studied using various spectroscopic techniques, UV/visible, fluorescence, time-resolved fluorescence, circular dichroism, FTIR, etc. The experimental findings were validated by molecular docking. We evaluated CFNPs as agents for photothermal therapy and magnetic hyperthermia therapy. CFNPs were coated with a layer of silica and it was loaded with a photosensitizer. The photosensitizer gave photodynamic therapy and gave the nanoparticles the potential to be used for combination therapy. The interactions of CFNPs were studied with another model protein, lysozyme. The favorable interactions take the nanoparticles a step further in clinical use.

*Contents*

1. Introduction 2. Literature Review 3.Experimental and Characterization Techniques 4. Doxorubicin loaded casein nanoparticles; synthesis, characterization, and in *vitro* evaluation 5. Cobalt ferrite nanoparticles for magnetically induced thermal therapy, and their biological interactions with lysozyme 6. Methylene blue silica coated cobalt ferrite nanoparticles with potential for combination therapy 7. Manganese ferrite nanoparticles; synthesis, characterization, and its biological interactions with bovine serum albumin employing spectroscopic and molecular docking techniques 8. Conclusion. Research publications and Conference certificate.

09. GOSWAMI (Neha)
**Modular Theory for Local and Global Admittance of Rough/Modified Electrode, Solid Electrolyte and Li-Ion Cell.**
Supervisor : Prof. Rama Kant
Th 25044

*Abstract*
*(Not Verified)*

In this thesis we have developed a modular theoretical approach to explain the global electrochemical impedance behavior of following complex systems: (i) solid electrolytes, (ii) electroactive thin film coated electrode and (iii) all solid state Li-ion cell. Another issue of importance in these systems is their interfacial stability and non-uniform growth during operation. This difficult problem is addressed through novel theoretical approach based on local electrochemical impedance spectroscopy (LEIS) developed for the diffusion controlled (reversible) charge transfer process under the influence of DC-bias potential, ohmic losses accounting the migration governed compact-electric double layer formation which is a prerequisite for charge transfer process. This approach assists in investigating the influence of multi-scale (fractal) roughness of electrode on non uniform local growth velocity. Theory for LEIS also accounts for migration correction to the local growth velocity. The complex electrochemical systems are usually unworkable and demand high degree of approximations in traditional theoretical and mathematical approaches. Therefore, we developed a modular theoretical approach in which the electrochemical system is partitioned into various interfacial modules and the constitutive equation for each module is derived through the phenomenological ab-initio approach. The overall impedance of the system is obtained by superposition of dynamic impedance of these interfacial modules. Modular theoretical approach has rigor of phenomenological ab-initio methodology as well as it allow us to capture the simplicity of equivalent circuit models. Modular theoretical approach provides deeper physical insights into the phenomenological intricacies of the complex electrochemical systems. This approach allows identifying the different frequency regimes in the impedance response of the system and the underlying governing phenomena unraveling the associated phenomenological time and length scales. To prove the validity of this modular approach theoretical results are also corroborated with the experimental data.

*Contents*

1. Introduction to phenomena in liquid and solid electrochemical interfaces 2. Theory for DC bias admittance based diffusion limited growth velocity at rough electrode 3. Theory for DC bias admittance based local growth velocities under the influence of diffusion, solution resistance and electrode roughness 4. Modular theory for DC bias admittance response of electroactive film modified electrode 5. Modular theory for impedance response of solid state electrolyte 6. Modular theoretical approach for impedance of all solid state Li-ion cell 7. Summary and future perspective.

10. GULATI (Archa)
**Removal of Noxious Water Pollutants by Using First Row Transition Metal Oxides as Efficient Heterogeneous Catalysts.**
Supervisor : Prof. Rita Kakkar
Th 25071

*Abstract*
*(Verified)*

The research work embodied in this thesis includes the synthesis, characterization and applications of first row transition metal oxides for the effective removal of toxic organic pollutants present in wastewaters by heterogeneous catalysis. Heterogeneous catalysis has emerged as an excellent method for the removal of pollutants owing to its ease of operation, effectiveness and remarkable regeneration and recyclability of the catalyst. Materials that can act as efficient heterogeneous catalysts should possess features such as (i) high surface area, (ii) facile synthesis, (iii) environmental benignity, (iv) robustness for continuous use, (v) low synthesis cost, and (vi) efficient regeneration and recyclability. Transition metal oxides are hence an excellent choice as catalysts since they possess all these characteristics.Precious transition metals such as Pd, Pt, Au and Ag have been extensively used in various catalytic reactions but their high cost and low abundance limit their use. Recently, the earth-abundant first row transition metals-based oxides have acquired formidable attention in the field of nanocatalysis and have emerged as alternatives for precious metals owing to their low cost, relatively less toxicity, enormous surface area, high availability and unique reactivity profiles. Also, oxone (2KHSO5.KHSO4.K2SO4) and sodium borohydride (NaBH4) are the favored, green, water soluble oxidant and reductant, respectively. They have been extensively used for the oxidative and reductive degradation of noxious organic water pollutants into harmless compounds.In the present study we have synthesized various first row transition metal oxides and studied their application in the removal of hazardous organic pollutants in combination with oxone/ NaBH4. We have also elucidated various factors like effect of concentration, catalyst dosage, contact time and temperature on the catalysis. The results indicate that first row transition metal oxides can be successfully employed as catalysts for the removal of toxic water pollutants and have huge potential as catalysts.

*Contents*

1. Transition metal oxides: excellent heterogeneous nanocatalysts for water remediation 2. Experimental techniques 3.Peanut shell biotemplate to fabricate porous magnetic $Co_3O_4$ coral reef and its catalytic properties for p-nitrophenol reduction and oxidative dye degradation 4.Bio-template cotton to synthesize mesoporous NiO and its catalytic properties for advanced oxidative dye degradation 5.Synthesis of hierarchically porous sphere-like CuO from a renewable mineral and its catalytic properties for p-nitrophenol reduction and oxidative degradation of caffeine 6. Mesoporous rGO@ZnO composite: Facile synthesis and excellent water treatment performance by catalytic by oxidative dye degradation 7. Conclusions and perspectives. Bibliography.

11. GULATI (Upasana)

**Design and Development of Coinage Metal (Cu and Ag) Nanocatalysts for Green and Sustainable Synthesis of Heteroatom Containing Value Added Molecules.**

Supervisor : Prof. Diwan S. Rawat

Th 25064

*Abstract*

*(Not Verified)*

Chapter 1A deals with magnetically recoverable CuO/Fe2O3 nanocatalysts (MRNCs) synthesized by the one-pot process of stabilizing CuO on hematite nanoparticles (NPs). The catalytic potential of CuO/Fe2O3 NPs was analyzed for synthesis of tri/tetra substituted propargylamines via. decarboxylative one-pot A3/KA2 reaction. Chapter 1B: Here, we have extended the scope of A3 reaction to synthesize pyrrolo[1,2-a]quinolone heterocycles. The reaction was catalyzed by Cu/HM nanocatalyst, obtained by stabilizing copper on magnesium mineral, hydromagnesite which served as support as well as base catalyst. Further, Cu/HM is calcined to obtain CuO/MgO nanocatalyst which is utilized for the synthesis of iminochromenes via. “click and activate” mechanism. Both the catalyst showed excellent activity, recyclability and ideal green chemistry metrics.Chapter 2A, porous Cu@SiO2

nanospheres (NSs) are prepared by an environmentally benign process. The obtained Cu@SiO2-NS served as versatile nanocatalyst for the synthesis of aminoindolozines, pyrrolo[1,2-a]quinolones, and substituted pyrrolidine. Chapter 2B: Reduced graphene oxide supported copper oxide (RGO@CuO) nanocomposites (NCs) was synthesized and its activity is explored for the synthesis of α-alkynylated N-substituted pyrrolidines.Chapter 3A deals with reduction of RGO@CuO-NCs to RGO@CuI-NCs which is found to be robust catalyst for aerobic and anaerobic single electron transfer (SET) reactions. The nanocatalysis study outlines two distinct mechanistic pathways for aerobic and anaerobic SET reactions. Chapter 3B: Magnetically recoverable Ni@CuI hybrid nanocatalysts was obtained by oxidation of Ni@Cu core-shell precursor. The nanocatalyst showed high catalytic activity, broad substrate scope and excellent recyclability for synthesis of value-added spiropyrrolines molecules.Chapter 4: Here we developed a 3D porous MgO framework with Ag0 nanoparticles for ambient pressure activation and insertion of CO2 into unsaturated alkyne substrates. The catalyst is effective for conversions of challenging CO2 feedstock with excellent recyclability (5×).

*Contents*

1A. Robust and magnetically recoverable $CuO/Fe_2O_3$ Nanocatalyst for decarboxylative A3 and KA2 coupling reactions 1B. Hydromagnesite derived Cu/HM and CuO/MgO Nanocatalysts for the synthesis of tetrasubstituted propargylamines and isochromenes 2A. Mesoporous silica nanosphere supported copper oxide ($CuO/SiO_2$) for the synthesis of N-heterocycles via decarboxylative coupling strategy 2B. Reduced graphene oxide supported copper oxide (RGO@CuO) nanocomposites from copper mineral precursor: A green approach for decarboxylative activation of proline amino acid to afford value-added synthons 3A. RGO@Cul manocomposite for aerobic and inert single electron transfer (SET) reaction for the synthesis of benzimidazole and spiropyrroline heterocycles 3B. Designing of bimetallic magnetic Ni@Cul hybrid nanodimer: cooperative catalytic activation of olefins and oximes to afford spiropyrroline heterocycles 4.MgO@Ag hybrid interfacial nanocatalyst for ambient $CO_2$activation to afford ester and lactone heterocycles.Summary, List of publications, Honours & awards, Conferences etc.

12. GUPTA (Jyoti)
**Physicochemical Studies of Interactions of Selected Amino Acids in Aqueous-Drug Media.**
Supervisor : Dr. Anil Kumar Nain
<u>Th 25078</u>

*Abstract*
*(Not Verified)*

The first chapter of this thesis is an introductory chapter. It comprises of objective, significance and scope of proposed work. Various experimental techniques used for the measurements of density, speed of sound and viscosity at different temperatures are dealt in the second chapter. Chapter 3 summarizes the densities, $\rho$, speeds of sound, $u$ and viscosities, $\eta$of aqueous streptomycin sulphate solutions *i.e.*, in water and in aqueous *l*-asparagine/*l*-glutamine solvents at different temperatures. Chapter 4 comprises of experimental values of densities, speeds of sound and viscosities of glycine/*l*-alanine/*l*-valine/*l*-isoleucine with aqueous-isoniazid solvents at six temperatures. In chapter 5, we have scrutinised the molecular interactions occurring in the systems by measuring densities, $\rho$, speeds of sound, $u$ and viscosities, $\eta$for gentamicin sulphate in water and in aqueous *l*-asparagine/*l*-glutamine solvents. The aim of chapter 6 is evaluation of volumetric, acoustic and viscometric properties of polar amino acids *l*-arginine and *l*-histidine in aqueous and aqueous-sodium salicylate. In chapter 7, reliable thermophysical data is reported by measuring $\rho$, $u$ and $\eta$of glycine/*l*-alanine/*l*-valine/*l*-isoleucine in aqueous-semicarbazide hydrochloride. In chapter 8, physicochemical properties and the nature of interaction of amino acids in aqueous semicarbazide hydrochloride have been scrutinized.

*Contents*

1. Introduction 2. Experimental methods 3. Drug- amino acid interactions in aqueous-medium: thermodynamic and transport properties 4. A quest on the concept of kosmotronicchaotropic behaviour of homologous series of α-amino acids in aqueous-isoniazid solutions 5. Molecular interactions of gentamicin sulphate in aqueous-*l*- asparagine/*l*-glutamine solutions at different temperatures: Thermo-acoustic and rheological properties 6. Study to reconnoiter solvation consequences of *l*-arginine/l-histidine and sodium salicylate in aqueous environment probed by physicochemical approach 7.Effect of concentration and temperature on apparent molar properties of homologous α-amono acids in aqueous-semicarbazide hydrochloride solutions 8. A link between physicochemical properties and non-covalent interactions involving *l*-arginine and *l*-histidine: The effect of charge on π-π stacking with hydrotropic agents. List of publications.

13. GUPTA (Mohit)

**Palladium-Catalyzed C-H Functionalization of 2-phenyl-4H-Benzo[d][1,3]oxazin-4-ones.**

Supervisor : Dr. B. K. Singh

Th 25029

*Abstract*
*(Not Verified)*

The work presented in Chapter I entitled “Palladium-Catalyzed Regioselective Acyloxylation of 2-phenyl-4H-Benzo[d][1,3]oxazin-4-ones” describes an efficient, and practical method for the direct regioselective ortho-acyloxylation of 2-phenyl-4H-benzo[d][1,3]oxazine-4ones using palladium acetate as a catalyst and PhI(OAc)2/ PhI(OCOtBu)2 as an acyloxy source.In the present chapter, we have developed a palladium-catalyzed simple and practical method for the direct regioselective ortho-acyloxylation using PhI(OAc)2/ PhI(OCOtBu)2 as acyloxy source. The method exploits the nitrogen of heterocyclic ring to assist the regioselective C-H activation of benzene at ortho-position via the formation of the palladacycle intermediate. Nevertheless, the established method has wide substrate scope, high functional group tolerance and delivers all the products synthesized in good yields to moderate yields.The work presented in Chapter II entitled “Palladium-Catalyzed C-H Functionalization and Subsequent Annulation of 2-phenyl-4H-Benzo[d][1,3]oxazin -4-ones using Aroyl Surrogates” describes an efficient approach for the synthesis of 6a-phenyl-5H-benzo[4,5][1,3]oxazino[2,3-a]isoindole-5,11(6aH)-diones using abundantly and easily available substrates such as toluenes, aldehydes and benzyl alcohols as reaction partners.The work presented in Chapter III entitled “Palladium-Catalyzed decarboxylative ortho-Aroylation and Subsequent Annulation of 2-phenyl-4H-Benzo[d][1,3]oxazine-4-ones” describes a highly efficient, palladium catalyzed synthetic approach for the synthesis of 5H-benzo[4,5][1,3]oxazino[2,3-a]isoindole-5,11(6aH)-diones using a-oxo carboxylic acid as aroyl surrogate. Isoindolinones are an important class of heterocycles in organic chemistry. This moiety forms an essential structural motif of many biologically significant molecules, natural products and useful intermediates in the synthesis of several drug-like molecules.

*Contents*

1. Palladium-vatalyzed regioselective acyloxylation of 2-phenyl-4H-Benzo[d][1,3] oxazin-4-ones 2. Palladium-catalyzed C-H functionalization and subsequent annulation of 2-phenyl-4*H*-benzo[d][1,3]oxazin-4-ones using aroyl surrogates 3. Palladium-catalyzed decarboxylative *ortho*-aroylation and subsequent annulation of 2-pheyl-4*H*-benzo[d][1,3]oxazine-4-ones. Summary.

14. GUPTA (Radhika)
**Design, Synthesis and Application of Recyclable Ionic Liquids Supported Silica-based Magnetic Nanocatalysts for Various Organic Transformations.**
Supervisor : Prof. R. K. Sharma
Th 25032

*Abstract*
*(Verified)*

In the present research work, we have designed, fabricated and characterized novel ILs supported magnetically retrievable nanocatalysts with an objective to conduct organic reactions with credentials such as high efficiency, economic viability, non-toxic and mild reaction conditions, catalytic reusability and opportunity towards large scale industrial applications. The present work has been divided into six chapters. Chapter one exhaustively summarizes the most recent advances in the development of magnetically supported ionic liquids reported in the field of catalysis. Chapter two provides a comprehensive overview of the advanced spectroscopic and microscopic techniques that have been employed for the characterization of different nanomaterials and compounds synthesized throughout the work such as FT-IR, XRD, FE-SEM, TEM, VSM, XPS, GC-MS, NMR, etc. Chapter three describes the development of novel acetate-based butylimidazolium ionic liquid immobilized silica-coated magnetic nanoparticles for the synthesis of N-aryl-2-oxazolidinones under metal-, ligand- and solvent-free conditions. Chapter four elucidates the fabrication and characterization of silica-coated magnetic nanoparticles supported acid-functionalized DABCO-based ionic liquid for the synthesis of various bioactive 3,3-di(indolyl)indolin-2-ones. Chapter five illustrates the design and fabrication of a copper metal-containing IL immobilized silica-coated magnetic nanocatalyst which was further utilized for the tandem cyclization and oxidative synthesis of 2-phenylquinazolin-4(3H)-ones. Chapter six illustrates the fabrication and characterization of silica-coated magnetic nanoparticles supported imidazolium molybdate ionic liquid as an efficient nanocatalyst for conducting one-pot tandem oxidative synthesis of asymmetric imines from benzyl alcohols and amines under aerobic conditions. The reaction protocols established throughout the work approach the principles of green chemistry in terms of lesser waste production and milder reaction conditions. Besides, excellent product yields were obtained in each case under the assistance of catalytic materials which are easy to recover and recycle.

*Contents*

1. Introduction 2. Theory of instrumentation techniques used 3. Fabrication of $Fe_3O_4$@$SiO_2$-supported acetate-based butylimidazolium ionic liquid nanocatalyst for the straightforward one-pot synthesis of bioactive *N*-aryl-2-oxazolidinones under metal-and solvent-free conditions 4. Silica-coated magnetic nanoparticles supported DABCO-derived acidic ionic liquid for the efficient synthesis of bioactive 3,3-di(indolyl)indolin-2-ones 5. Silica-coated magnetically retrievable copper ionic liquid nanocatalyst for cyclooxidative synthesis of 2-phenylquinazolin-4(3*H*)-ones 6. $Fe_3O_4$@$SiO_2$ immobilized imidazolium molybdate ionic liquid: A high performance

heterogeneous catalyst for tandem oxidative synthesis of asymmetric imines. Summary, Spectral data and List of publications.

15. GUPTA (Shalu)

**AIEE Active Novel Quinoxaline and Pyridopyrazine Derivatives and their Applications as Metal Ion and Acid Sensors.**

Supervisor : Prof. Marilyn Daisy Milton

Th 25049

*Abstract*

*(Not Verified)*

Several novel quinoxaline and pyridopyrazine derivatives were designed and synthesized in good yields by using various reactions like Suzuki cross coupling, condensation and Heck coupling reactions. All the synthesized novel compounds were characterized by 1H NMR, 13C NMR, HRMS and IR spectroscopy. Few compounds were also characterized by single crystal X-ray diffraction spectroscopy. All the synthesized compounds displayed aggregation induced emission enhancement characteristics in mixed solvents upon increasing water fraction. The photophysical studies revealed that the intramolecular charge transfer was occurring from biphenyl donor to quinoxaline or pyridopyrazine acceptor. In order to fine tune the intramolecular charge transfer characteristics, groups of varying electronic nature were introduced on quinoxaline acceptor. Also, the intramolecular charge transfer characteristics were fine-tuned by modifying electron donor. Pyridopyrazine derivatives displayed selective and reversible detection of Hg2+ ions in the presence of other competitive metal in aqueous media. Compounds with electron withdrawing group showed "turn-on" and with electron donating group showed "turn-off" response towards Hg2+ ion. The detection limits were found in submicromolar range. For practical application, paper strips for mercury ion sensing were also constructed. Further, quadrupolar quinoxaline and pyridopyrazine based push-pull molecules were also used for volatile acid sensing in solution as well as in solid state. Quinoxaline based benzothiazoles displayed nitroaromatic explosive sensing in organic as well as in aqueous media. Also, acidochromism of quinoxaline based push-pull molecule was utilised to achieve white light emission in solution. Further, quinoxaline and pyridopyrazine based push-pull molecules with extended conjugation displayed linear dependence of emission maxima on temperature.

*Contents*

1. Introduction 2. Synthesis of novel Y-shaped AIEE active pyridopyrazines and their applications as chromogenic and fluorogenic probes for $Hg^{2+}$ detection in aqueous media 3A.Design and synthesis of novel Y-shaped AIEE active quinoxalines for acidochromic applications 3B. Y-shaped AIEE active quinoxaline-benzothiazole conjugate for fluorimetric sensing of nitroaromatic in aqueous media 4. Designing of novel AIEE-TICT active Y-shaped push-pull quinoxaline derivatives displaying solvatochromic and acidochromic applications 5. Novel Y-shaped push-pull quinoxaline detivatives: design, synthesis, AIEE and acidochromism 6. Design and synthesis of novel Y-shaped AIEE-TICT active quinoxalines with extended conjugation and their applications 7. Summary and conclusion, List of publications.

16. GUPTA (Shilpa)

**Molecular Dynamics Simulations of Poly (Propylene Imine) Dendrimer and its Polyelectrolyte Complexes in Dilute Solutions.**

Supervisor : Prof. Prabati Biswas

Th 25039

*Abstract*
*(Not Verified)*

Dendrimers are symmetrically branched tree-like monodisperse structures. Their structural properties may be influenced by the generations of growth, spacer lengths, solvent quality, and pH of the solution. The applications of dendrimers as guest transport vehicles are determined bytheir structural rearrangement. Such rearrangement alters the dynamic properties of dendrimers at different length and time scales. The investigation of conformations and dynamics of dendrimers is crucial for understanding their physical behavior and their interactions with the environmentand other molecules. This thesis investigates the internal structure and orientational dynamics of poly(propylene imine) (PPI) dendrimers as a function of pH through molecular dynamics (MD) simulations in dilute solutions. A conformational transition of PPI dendrimers is observed from anexpanded structure at low pH to a highly compact one at high pH. The orientational relaxation dynamics of these dendrimers is characterized by various correlation functions corresponding to different time and length scales. The conformations of PPI dendrimers at different pH conditionsin an ionic liquid (IL), 1-butyl-3-methylimidazolium chloride ([BMIM]Cl) are investigated. The lower generation dendrimers exhibit a conformational transition as a function of pH, while the higher generations exhibit a highly compact structure at all solution pH. PPI dendrimers in ILsexhibit more dense structure at neutral and low pH as compared to that in an aqueous medium. Dendrimers may be used as nanocarriers in biology, pharmacy, and medicine as complexes with polyelectrolytes. A simulation study is performed to study the conformational properties of PPIdendrimer polyelectrolyte complexes. The effect of chain length and charge of the polyelectrolyte chain on the formation of these complexes is studied as a function of the generations of growth. The simulation results presented in this thesis may be used to investigate the encapsulation orrelease of specific guest molecules for dendrimers and their complexes in different environments.

*Contents*

17. GYANENDRA KUMAR
**Synthesis of Metal Organic Frameworks and Graphene Based Nanocomposites for Drug Delivery and Catalytic Applications.**
Supervisor : Prof. Prabati Biswas
Th 25027

*Abstract*
*(Not Verified)*

The present thesis aims to contextualize the design and synthesis of three important functional materials; (1) Graphene-based nanocomposites and (2) Metal-organic framework-based nanocomposites (3) the Development of Graphene and Metal-organic framework nanocomposite materials. Briefly, a systematic investigation has been performed on these materials to explore their easy synthetic methods and their potential applications in the field of drug delivery and heterogeneous catalysis. Substantial progress has been seen in the design and synthetic methodology for

graphene-based nanocomposites and metal-organic framework but inexpensive percussors in environmentally benign reaction conditions to attain sustainable low-cost protocols are still required. The as-synthesized nanocomposites were characterized by FTIR, TGA, XRD, SEM, TEM, XPS, BET, ICP-OES, UV-visible spectroscopy, and Raman spectroscopic Techniques. Furthermore, the applications in organic reactions were investigated by Nuclear Magnetic Resonance (NMR) studies. The thesis has been comprised of seven chapters and the chapter-wise summary is given below.Chapter 1 deals with the general introduction to metal-organic frameworks and graphene-based nanocomposite materials. The critical literature review of these functional materials includes their characteristics properties, historical background, and their applications in drug delivery and catalysis.Chapter 2 covers the synthesis of MOF-5 and is used in the oral drug delivery system.Chapter 3 includes the synthesis and characterization of NiO nanocomposites immobilized on the surface of rGO nanocomposite material for the synthesis of imidazole derivatives.Chapter 4 includes the synthesis and characterization of Zr-based metal-organic framework/Reduced graphene oxide composites for the synthesis of 2,3-Dihydroquinazolin-4(1H)-one derivatives.Chapter 5 presents the synthesis and characterization of sustainable synthesis of MOF-5@GO-based nanocomposites for efficient removal of RhB from water.Chapter 6 presents the synthesis of chitosan/graphene oxide-based bio-nanocomposite beads and used as a drug carrier. As-synthesized Chi/GO beads have been utilized as a drug carrier for oral drug delivery of MTD drug.Chapter 7 Includes the summary and conclusions.

*Contents*

1. Introduction 2. Synthesis, characterizations and kinetic study of metal organic framework nanocomposite excipient used as extended-release delivery vehicle for an antibiotic drug 3. NiO nanocomposites/rGO as heterogeneous catalysis for imidazole scaffolds with their applications in inhibiting DNA binding activity 4. Zr-based metal organic framework/reduced graphene oxide composites for catalytic synthesis of 2,3-dihydroquinazolin-4-(1H)-one derivatives 5. Sustainable synthesis of MOF-5@GO nanocomposites for efficient removal of rhodamine B from water 6. Extended-release of metronidazole drug using chirosan/graphene oxide bio-nanocomposite beads as drug carrier 7. Conclusion and future aspects.List of publications and Conferences.

18. HEMANT KUMAR

**Preparation and Characterization of Inorganic Nanomaterials for Biomedical and Catalytic Applications.**

Supervisor : Prof. Balram Pani

Th 25033

*Abstract*
*(Not Verified)*

The aim of the present thesis is to contextualize the design and synthesis of inorganic nanomaterials. The research involved a simple production technique and its potential uses in biomedical applications and heterogeneous catalysis. It places a strong emphasis on the physicochemical characteristics of nanoparticles that have been chemically modified. FeS NCs outperform in comparison to previously reported heterogeneous and homogeneous catalytic techniques in terms of activity. Within two minutes, these nanoclusters were created. They are ferromagnetic, with a high magnetism (20 emu/g), and can be reused up to five times without losing effectiveness for the production of 9-aryl-1,8dioxooctahydroxanthenes and 14-substituted-14H-dibenzo. The large surface area and porous structure of silica nanocomposites have gained a lot of interest for their application in the delivery of drugs. In this study, mesoporous silica encapsulated iron oxide (IO) nanocomposites loaded with doxorubicin (DOX) an anticancer drug was synthesized. This DOX/IO@Silica can be used for magnetically guided delivery of an anticancer drug, and can also be used as a contrast agent. The release pattern of a drug-loaded onto nanocomposites with an average size of 120 nm was studied and more than 83% (at pH = 5.4) optimal release of the drug was observed in two weeks. Another composite material Dox encapsulated silica nanoparticles (Dox@Si) were synthesized and was coated with folic acid to get FA/Dox@Si, as it can be easily recognized by cancer cells and they can efficiently deliver more drugs compared to free Dox. The shape, size, morphology, crystallinity, porosity, and functionalization were analyzed by using several characterization techniques, such as DLS, TEM, and FTIR. The drug release pattern was recorded for 15 days, which showed sustained and regulated release of drug from the mesoporous silica nanocomposite.

*Contents*

1. Introduction 2. Experimental and characterization techniques 3. Mono dispersible water-soluble iron sulphide nanoclusters: synthesis, characterization and catalytic application for highly efficient synthesis of xanthene derivatives 4. In-vitro and bio-imaging studies of mesoporous silica nanocomposites encapsulated iron-oxide and loaded doxorubicin drug (DOX/IO@ silica) as magnetically guided drug delivery system 5. Multifunction folic acid coated mesoporous silica and doxorubicin encapsulated nanocomposites (FA/DOX@sulica for superior active targeting cancer therapeutics, bio-imaging and *in-vitro* studies 6. Conclusions & future aspects.List of publications and Conferences.

19. JOGENDER

**Adsorption of Halogenated Compounds and Gases on Small Metal Cluster Decorated Graphene Surfaces: DFT-D2 Studies.**

Supervisor: Prof. Rita Kakkar

Th 25032

*Abstract*
*(Verified)*

In this thesis, we studied the adsorption of various halogenated compounds and gases on pristine graphene and small metal cluster decorated graphene surfaces. Overall, the thesis is divided into seven chapters. A brief outline is provided below.Chapter 2 (Computational Techniques) describes the various computational techniques used in this work. Density Functional methods are described, as also the details of basis sets, convergence criteria, different k-point sets and principles involved in adsorption.Chapter 3 (Decontamination of Chloropicrin (PS) and its Analogues using Graphene and Modified Graphene Surfaces: A Computational Study) includes the adsorption of chloropicrin and its analogues on different graphene surfaces.Chapter 4 (A DFT-D2 Study on the Adsorption of Phosgene Derivatives and Chloromethyl Chloroformate on Pristine and Fe4-decorated Graphene), pristine graphene and Fe4 decorated graphene surfaces have been used for the adsorption of phosgene, diphosgene, phosgene oxime and chloromethyl chloroformate (CMCF).Chapter 5 (Adsorption of Methyl Isocyanate on M4 (M = Fe, Ni and Cu) Cluster-decorated Graphene and Vacancy Graphene: A DFT-D2 Study) describes the adsorption of methyl isocyanate (MIC) on various graphene surfaces modified by decoration of Fe4, Ni4 and Cu4 tetramer clusters on pristine graphene.Chapter 6 (A DFT-D2 Study on Mo4-xCox (x = 0 - 3) Cluster Decorated Graphene and the Adsorption of SO2F2 and SOF2 on Mo4 Decorated Graphene), mixed tetramer clusters of Mo and Co were adsorbed on pristine graphene. The adsorption of SO2F2 and SOF2 gas was further studied on the Mo4- decorated graphene.Chapter 7 (Conclusions), a few concluding remarks are presented and the scope for future work is given.

*Contents*

1. Recent advances on graphene-based gas sensors 2.Computational techniques 3. Decontamination of chloropicrin (PS) and its analogues using graphene and surfaces: a computational study 4. A DFT-D2 study on the adsorption of phosgene derivatives and chloromethyl chloroformate on pristine and $Fe_{4-}$ decorated graphene 5. Adsorption of methyl isocyanate on $M_4$ (M = Fe, Ni and Cu) cluster-decorated graphene and vacancy graphene: a DFT-D2 study 6. A DFT-D2 study on $Mo_{4-x}$ $Co_x$ (x = 0 – 3) cluster decorated graphene and the adsorption of $SO_2F_2$ and $SOF_2$ on $Mo_4$ decorated graphene 7. Conclusions and Bibloigraphy.

20. JOSHI (Akanksha)

**Design and Assessment of Defects Rich Electrodes for Supercapacitive Charge Storage.**

Supervisor : Prof. Raj Kishore Sharma

Th 25050

*Abstract*
*(Verified)*

To unveil the role of active sites is of large significance for the design and development of high performance electrode materials. Defects in the form of vacancies and edges act as charge storage active sites and are not considered as aimperfections. These defects have the ability to modulate electronic, surface and electrochemical properties. In the entire work, different type of defects mainly vacancy and edges are introduced either individually or in combination for high performance supercapacitive properties. In one work, MoO3 nanoflowers are encapsulated into the defect rich activated carbon for synthesis of negative electrode for supercapacitor. The edges of nanoflower offer plenty of active sites for charge storage. Then in another work vacancies are deliberately introduced to act as active sites and modulate both electronic and electrochemical properties. Afterwards, oxygen defects are introduced into the boron nanosheet structure that stabilizes the structure in aqueous electrolytes. In the last work, multiple defect vacancy and edges both are introduced in one step into the Ni3S2, which not only improves conductivity (one order) and large carrier concentration but also further augments energy density and cyclic stability. Based on their electrochemical study, introduction of multiple defect rather than individual defect has found to be most effective method in enhancement of supercapacitive performance.

*Contents*

1. Introduction: role of defects in supercapacitivecharge storage materials 2.Synthesis and characterization to create and identification of defects 3. Defect rich activated carbon support for $MoO_3$ nanoflowers: a high performance supercapacitor negative electrode 4. Flexible, sustainable and high performance supercapacitor from oxygen deficient, bimodal mesoporous silica5.Stabilizing complex bonding structure of boron of nanosheet through oxygen defect: an approach for high-performance supercapacitor 6. Active sites exposure through multiple defects towards enhancement of $Ni_3S_2$ charge storage characteristics 7. Conclusion.Appendix and List of publications.

21. KAIM (Vishakha)

**Synthesis, Characterization and DFT Studies of Mono-/Di-nuclear Mn and Ru Complexes for Electrocltalytic Proton Reduction.**

Supervisor : Dr. Sandeep Kaur

Th 25059

*Contents*

1. Introduction 2. Dinuclear manganese carbonyl complexes: electrocatalytic reduction of protons to dihydrogen 3. Hydrogen evolution reaction catalysed by mononuclear Mn Complexes: an experimental and theoretical study 4. Mononuclear Mn complexes featuring N, S-/N, N-donor and 1,3,5-triaza-7-phosphaadamantane ligands: synthesis and electrocatalytic properties 5. Mononuclear ruthenium phosphine complexes: synthesis, DFT calculation and electrocatalytic hydrogen evolution 6. Synthesis, characterization and electrocatalytic properties of mononuclear RU(II complex [*cis*-$RuCl_2(PPh_3)_2(k^2\text{-}TL_6)$] ($TL_6$ = 2-thiophenylbenzimidazole). Summary and conclusion, List of publications.

22. KASHYAP (Kriti)

**Achieving Selective Inhibition of Histone Deacetylase Isoforms : An in silico Approach.**

Supervisor : Prof. Rita Kakkar

Th 25077

*Abstract*
*(Verified)*

Histone deacetylases (HDACs) are a family of eleven zinc-dependent epigenetic modulators responsible for the removal of acetyl groups from post-translationally modified lysine residues of histone proteins. They play a crucial role in regulation of gene expression by deacetylating the acetylated lysine residues and restoring the DNA to its transcriptionally inactive state. HDACs also regulate the activity of non-histone protein substrates like α-tubulin, actin and other proteins involved in cell-signaling, apoptosis, DNA repair and replication. Overexpression of HDAC isoforms leads to suppressed transcription and gene silencing. Often, expression of tumor suppressor genes is silenced due to abnormal HDAC activity. Recently, HDAC inhibitors have been reported to have anti-tumor activity, with four HDAC inhibitors being approved for treatment of various lymphomas. However, they have the disadvantage of being pan-inhibitors, i.e., they inhibit multiple isoforms simultaneously. Since, HDACs play important roles in crucial physiological processes, pan-inhibition has resulted in many off-target side-effects being reported. Therefore, efforts are now focused towards the development of isoform-selective inhibitors. The research work presented in this thesis comprises in silico studies of the histone deacetylase (HDAC) enzyme family and its inhibitors. In the first study (Chapter 3), induced-fit docking of a highly selective HDAC8 ligand library has been carried out, followed by generation of pharmacophore-QSAR models that highlight the structural features necessary for potent and selective inhibition of HDAC8. Highly selective HDAC8 lead molecules have been proposed in the next study (Chapter 4) by using these models as 3D queries in a virtual screening protocol. The next study (Chapter 5) is aimed at gaining an insight of the receptor-ligand interactions responsible for selective inhibition of the different HDAC isoforms through molecular docking studies of highly selective HDAC2, HDAC4, HDAC6 and HDAC8 ligands. In the last study (Chapter 6), the therapeutic effects of hybrid Topoisomerase-HDAC inhibitors have been explored.

*Contents*

1. Structural bases for selective inhibition in histone deacetylases : 2. Computational techniques 3. An insight into selective and potent inhibition of histone deacetylase 8 through induced-fit docking, pharmacophore modeling and QSAR studies 4. Lead identification and optimization for selective and potent inhibition of histone deacetylase 8 through pharmacophore-enabled virtual screening and molecular docking 5. Exploring structural requirements of isoform selective histone deacetylase inhinitors: a comparative in silico study 6. In silico study of the synergistic anti-tumor effect of hybrid topoisomerase-HDAC inhibitors 7. Concluding remarks. Bibliography.

23. KAUSHIK (Reetam)
**Organic-Inorganic Moieties as Templates/Linkers in the Synthesis of Lone Pair Containing Polyoxotungstate Clusters.**
Supervisor : Dr. Firasat Hussain
<u>Th 25042</u>

*Abstract*
*(Not Verified)*

The thesis entitled "Organic-Inorganic moieties as templates/linkers in the synthesis of lone pair containing polyoxotungstate clusters". Chapter I includes, introduction of polyoxometalates compounds, classification of POMs compounds and their applications. A key focus is put on the role played by the organic/inorganic moieties during the synthesis of the lone pair containing polyoxotungstates. In addition, a brief description of the instrumental techniques used for characterization such as FT-IR spectroscopy, Single crystal X-Ray diffraction, UV/Vis. Spectroscopy, Elemental analysis (ICP-AES), Field Emission Scanning Electron Microscopy, 13C-NMR and ESI-MS etc. is also given. Chapter II deals with the synthesis and characterization of three carbonate-encapsulated yttrium and ytterbium containing polyoxotungstates of the formula Na12[NaCH3COO{Y2(H2O)3 (AsW9O33)2 (W2O5)(CO3)}]·22H2O and [Ln3(A-β-GeW9O34)2(CO3)(H2O)3]13- {Ln = YIII, YbIII }. Chapter III deals with the synthesis and characterization of three inorganic-organic hybrid copper and cobalt containing arsenotungstates (III) with lone pair on heteroatom incorporating bidentate N donating ligands. The compounds are of the formula [NaRb{Cu(phen)(H2O)2Cl}2][{Cu(phen)(H2O)}2{Cu(phen)(H2O)Cl}2 {Cu2As2W19O67 (H2O), [NaRbCo(phen)3][{Co(phen)(H2O)3}CoAs2W20O67(H2O)3] and 2,2'-bipyridine [Na3RbCo(2,2'-bipy)3][CoAs2W20O67(H2O)3] which have synthesized under mild reaction conditions. Chapter IV deals with the synthesis eight rare earth containing antimonytungstates of the formula Na22[((RE)4(H2O)6Sb6O4)(SbW10O37)2(SbW8O31)2] [(RE)III = Y, Gd, Tb, Dy, Ho, Er, Tm, Yb] and their characterization by various analytical techniques.

*Contents*

1. Introduction, materials and methods 2. Synthesis and characterization of carbonate encapsulated ytterbium and yttrium containing polyoxotungstates 3. Synthesis and characterization of three inorganic-organic hybrid copper and cobalt containing arsenotungstates (III) with lone pair on heteroatom incorporating bidentate N donating ligands 4. Synthesis an characterization of $Na_{22}[(RE)_4(H_2O)_6Sb_6O_4](SbW_{10}O_{37})_2(SbW_8O_{31}))_2]$ $(RE)^{III}$ = Y, Gd, Tb, Dy, Ho, Er, Tm, Yb]. Conclusion of thesis. List of publications.

24. KHAN (Imran)
**Synthesis and Characterization of Octanuclear Lanthanide-Containing Silico and Germanotungstates and It's Catalytic Application for Oxidation of Alcohols.**
Supervisor: Firasat Hussain
Th 25563

*Abstract*
*(Not Verified)*

Chapter I includes, introduction of polyoxometalates compounds, Polyoxometalates (POMs) are metal-oxygen nanoclusters which consist of early transition metals such as Mo (VI), W (VI), V (V), etc. in their highest oxidation state. Due to the flexibility in their structure, size, charge density and redox potential, POMs show various interesting applications such as in the field of medicine, material science, catalysis, magnetism, clinical chemistry, photochemistry and analytical chemistry. Polyoxometalates (POMs) are metal-oxygen nanoclusters which consist of early transition metals such as Mo (VI), W (VI), V (V), etc. in their highest oxidation state. Due to the flexibility in their structure, size, charge density and redox potential, POMs show various interesting applications such as in the field of medicine, material science, catalysis, magnetism, clinical chemistry, photochemistry and analytical chemistry. Chapter II consists of syntheses of starting materials, Na10[A-α-GeW9O34]·18H2O,Na10[A-α-SiW9O34]·16H2O, Na8[HPW9O34]· 19H2O, K7 [HPW11O39]· 14H2O, K14[P2W19O69(H2O)]·24H2O and instrumental techniques used for characterization such as FT-IR spectroscopy, Single crystal X-Ray diffraction, UV/Vis. spectroscopy (Solid and Liquid), Photoluminescence spectroscopy, Elemental analysis (ICP-AES), Powder X-Ray diffraction, Gas Chromatography (GC) and ESI-MS. Chapter III deals with syntheses and characterization of a series of six lanthanide-containing germanotungstates of the formula: [(Ln2GeW10O38)4(W3O8)(OH)4(H2O)2]26- {(LnIII = Sm (1), Eu (2), Gd (3), Tb (4), Dy (5), Ho (6)}. Chapter IV consists of ten 1a - 10a silicotungstate nanoclusters with the molecular formula [(Ln2SiW10O38)4(W3O8)(OH)4(H2O)2]26− [LnIII = Sm (1), Eu (2), Gd (3), Tb (4), Dy (5), Ho (6), Er (7), Tm (8), Yb (9), and Y (10)]. Chapter V contains Comparative study of catalytic activity of tetrameric lanthanide-substituted polyoxotungstates [(Ln2XW10O38)4(W3O8)(OH)4(H2O)2]n− (X = SiIV, GeIV, PV and n = 26, 25) for the oxidation of alcohols.

*Contents*

1. Polyoxometalates and introduction 2. Experimental section 3. Self-assembled tetrameric lanthanide containing germanotungstates $[(Ln_2GeW_{10}O_{38})_4(W_3O_8)(OH)_4(H_2O)_2]^{26-}$: syntheses, crystal structure, photoluminescence and electrochemical properties 4. Tetrameric lanthanide-substituted silicotungstate $\{Ln_8Si_4W_{40}\}$ nanoclusters: syntheses, structural characterization and electrochemistry 5. Comparative study of catalytic activity of tetrameric lanthanide-substituted polyoxotungstates $[(Ln_2XW_{10}O_{38})_4(W_3O_8)(OH)_4(H_2O)_2]^{n-}$ (X = $Si^{IV}$, $Ge^{IV}$& $P^{V}$ and n = 26 or 25) for the oxidation of alcohols. Conclusion of the thesis, List of publications.

25. KRISHAN KUMAR
**Phase Transition of Thermoresponsive Polymer in Presence of Proteins as Stimuli.**
Supervisor : Prof. P. Venkatesu
Th 25031

*Abstract*
*(Not Verified)*

Thermoresponsive polymers (TRPs) have gained vast interest in scientific community because of promising applications in sensors, gels, drug delivery devices such as the nanops (nanostructured porous silicon), biotechnology and pharmacology. Chapter 3 reveals the thermally induced molecular conformational behavior of PVCL in the presence of three heme proteins Cyt c, Mb and Hb. The results from different biophysical studies demonstrate formation of protein-polymer mixed complex system which increases the lower critical solution temperature (LCST) of PVCL toward higher temperature with addition of heme proteins. Similarly, in chapter 4 we comparatively investigated the effect of heme proteins on thermal phase transitions of PNIPAM-b-PVCL block copolymer. Despite all the proteins belong to the heme group, different modifications observed in the LCST is due to different biomolecular interactions and structural arrangements of proteins. Moreover, the effect of heme proteins on the LCST transition of PNIPAM-b-PVCL is different for homopolymer PNIPAM and homopolymer PVCL. Sequentially, chapter 5 comprises of study of synthesizing and understanding phase transition behavior of three novel random (r) copolymers which are PVCL50-PDMAEMA50 PVCL30-PDMAEMA70 and PVCL70-PDMAEMA30. Time resolved fluorescence spectroscopy results demonstrate that copolymer PVCL50-PDMAEMA50 has slower fluorescence decay time when compared with other copolymers i.e. PVCL30-PDMAEMA70 and PVCL70-PDMAEMA30. Furthermore, the thermal phase transition in presence of insulin demonstrated the decrease in the LCST of co-polymer. Chapter 6 unveils the micellization behavior of well-known triblock copolymer poly(ethylene glycol)-block-poly(propylene glycol)-block-poly(ethyleneglycol) (PEG-PPG-PEG) in presence of two different proteins i.e. α-chymotrypsin (CT) and lysozyme (Lys). Currently, polymer-protein bio-conjugates are emerging as acceptable materials for applications in the fields of biomedical, drug delivery, protein separation and protein purification. Therefore, knowledge of the interactions between TRPs and protein is very important to fabricate these potential materials for protein adsorption through a phase transition.

*Contents*

1. Introduction and review of the literature 2. Materials and experimental techniques 3. Comprehensive insight into the protein-surface biomolecular interactions on a smart material: complex formation between poly(N-vinyl caprolactam) and heme protein 4. Biological stimuli-induced phase transition of synthesized block copolymer: preferential interactions between PHIPAM-b-PVCL and heme proteins 5. Insulin-induced conformational transition of fluorescent copolymer: a perspective of self-assembly between protein and micellar solution of smart copolymer 6. Role of protein-copolymer assembly in controlling micellization process of amphiphilic triblock copolymer 7. Conclusions.

26. MAIKHURI (Vipin Kumar)
**Novel Route to Chromanes & Chromenes from D-Mannose and Click Synthesis of Coumarinyltriazolylglycosides & 1,4-Disubstituted Triazoles.**
Supervisor : Prof. Ashok K. Prasad
Th 25058

*Abstract*
*(Verified)*

Chromanes and chromenes are widely distributed in nature and display a broad range of biological and pharmaceutical activities. Due to the biological importance of

chromane and chromene core, efforts have been made to develop an efficient and selective synthetic method to afford such molecules. Many methods are available for the synthesis of chromane moieties, but most of them use pertinently functionalized aromatic moiety as starting compound in order to annulate the pyran ring system. The chromane and chromene scaffolds has been synthesized from the carbohydrate moiety using palladium catalyzed cross dehydrogenative coupling reaction followed by subsequent 6π-electrocyclization and aromatization. The incremental frequency of resistance to active antifungal drugs and other antibiotics has elicited the growing public concern that the currently existing drugs would be inadequate in treating these infections. Many studies confirm that these currently available drugs to treat diseases have severe drawbacks, low efficiency rates and noxious side effects. Therefore, there is a vital requirement for new therapeutic agents with potency and broad spectrum activities. Organic scaffolds containing coumarin moiety displays a wide range of biological activities such as antimicrobial, anticancer, antiproliferative, antitumor, antioxidant, antiviral, etc. The coumarin as well as sugar moieties have broad range of applications and biocompatibility. Further, 1,2,3-triazoles are important class of N-heterocycles in medicinal as well as in organic chemistry. Connecting triazole with sugar and coumarin moiety could bring forth some interesting biological and photophysical properties. A series of coumarinyltriazolylglycosides and 1,4-disubstituted 1,2,3-triazoles has been synthesized in good to excellent yields. These compounds can be studied for the evaluation of their biological properties.

*Contents*

1. D-Mannose to chromane via pd-catalyzed cross dehydrogenative coupling and thermal cyclization 2. Novel synthesis of chromanes from 1,2-disubstituted glucal 3. Synthesis of coumarinyltriazolylglycosides via click reaction 4. Synthesis of novel 1,4-disubstituted triazoles. Summary, List of publications and Workshops and conferences.

27. MANOJ KUMAR
**Metal-Catalyzed C-H Functionalization of Arenes and their Mechanistic Investigation.**
Supervisor : Prof. Akhilesh K. Verma
Th 25040

*Abstract*
*(Verified)*

We have investigated copper-mediated direct ortho–C–H amination of arenes has been accomplished with the aid of easily removable bidentate pyridine N-oxide as a directing group. The use of free secondary amines and anilines as aminating agents, inexpensive copper acetate in external oxidant and additive–free condition makes the strategy more effective and favorable from the economic point of view. This reaction is compatible with a wide range of functional groups to synthesize a variety of amine-containing products of high interest. This method also allows the short synthesis of central scaffold of pharmaceutically relevant Staphylococcus aureus Sortase A inhibitor.The capture of reactive intermediates empowers chemists to conjecture the detail of a chemical transformation. Here we explore the mechanism of a C–H amination by intercepting short-lived intermediates in real time by online mass spectrometry. Computational study unravels the favorable pathway of the proposed dual mechanism of the reaction.Selective tandem oxidative C-H olefination-aza-Michael/aza-Wacker reaction of N-aryl benzamides is achieved by fine-tuning between base and additive to access valuable 3-oxoisoindolinyls and 3-

oxoisoindolinylidenes, respectively. Careful optimization and control experiments provides guiding principle in designing of a proposed catalytic cycle. The copper-iminium complex acting as a precursor for the binding of Ru catalyst was isolated and confirmed by X-ray diffraction. The versatility of this catalytic system has been demonstrated by the synthesis of biologically relevant molecules.Copper-catalyzed [3+2] cycloaddition of N-tosylcyclopropylamines has been accomplished under photoredox condition. Both akenes and alkynes can be used effectively coupling partner in the reaction to furnish corresponding aminated cyclopentanes and cyclopentenes, respectively.

*Contents*

1. Cu (II)-mediated ortho-C-H amination of arenes with free amines 2. Mechanistic insights of Cu(II)-mediated ortho-C-H animation of arenes by capturing fleeting intermediates and theoretical calculations 3. Ru(II)-oxidative olefination of benzamides: switchable aza-michael and aza-wacker reaction for synthesis of isoindolinones 4. Copper-catalyzed ring-expansion of protected cyclopropylamine with alkenes/alkynes in photo-redox medium. Summary and List of publications.

28. MANISH KUMAR

**Synthesis and Characterization of Metal Complexes based on Quinolone Derivatives and Heterocyclic Ligands for their Biological Applications.**

Supervisor : Dr. Dhanraj T. Masram

Th 25061

*Abstract*
*(Not Verified)*

The thesis entitled "Synthesis and Characterization of Metal Complexes based on Quinolone Derivatives and Heterocyclic Ligands for Their Biological Applications" is to design and synthesis of metal complexes based on quinolones for examining the different biological applications. CHAPTER 1 contain the brief introduction of quinolone derivatives and their biological properties, available in the literature. The aim of CHAPTER 2 is to synthesis and characterization of the copper(II) complexes with nalidixic acid or 2,2'-dipyridylamine. The biological applications (such as DNA, proteins binding and cytotoxicity) of the complexes were also investigated. The aim of CHAPTER 3 is to synthesis and structure characterization of the copper(II) complex with N-donor heterocyclic ligand 2,2′-dipyridylamine (bipyam) and results in the formation of [Cu(II)(bipyam)2Cl]. This complex interacts with serum albumins and DNA which have been studied by various techniques. The complex show potential cytotoxicity against MCF-7 cells. CHAPTER 4 describe the copper(II) complex with quinolone drug nalidixic acid and 2,2'-bipyridyl. The complex exhibited promising antibacterial activity against both Escherichia coli and Staphylococcus aureus. This complex has a superior ability to binds with DNA and proteins. Also, the complex showed potential cytotoxicity. CHAPTER 5 discuss the two cationic levofloxacin based copper(II) with their excellent binding interaction modes towards calf-thymus DNA and proteins were examined by a series of spectroscopy measurements. Molecular docking simulations were also employed to study the ability of the complexes to bind to these target macromolecules. Also, the complexes were subjected to cytotoxicity tests against MCF-7 cancer cell lines. The aim of CHAPTER 6 is to discuss the two new enoxacin based copper(II) complexes with their excellent binding and cleavage affinity towards DNA and proteins which explored by a series of spectroscopy techniques. The results of cytotoxicity suggested that complexes exhibit superior anti-cancer activity.

*Contents*

1. Introduction and review of literature 2. Structure, DNA/proteins binding, docking and cytotoxicity studies of copper(II) complexes with the first quinolone drug nalidixic acid nalidixic acid and 2,2'-dipyridylamine 3. Evaluation of DNA, and HAS ninding propensity of copper(II) complex with N-donor ligand 2,2'-bipyridylamine 4. Biological evaluation of copper(II) complex with nalidixic acid and 2,2'-bipyridine (bpy) 5. Copper(II) complexes based on levofloxacin and 2N-donor ligands: synthesis, crystal structures and in vitro biological evaluation 6. Copper(II) complexes containing enoxacin and hererocyclic ligands: synthesis, crystal structures and their biological perspectives. List of publications.

29. MANISH KUMAR
**Theories for DC Biased Impedance and Admittance Voltammetry at Fractally Rough Electrode: Diffusion, Adsorption and Coupled Catalytic Reactions.**
Supervisor : Prof. Rama Kant
Th 25035

*Abstract*
*(Verified)*

We have developed theories for DC biased electrochemical impedance and admittance voltammetric techniques for the processes involving diffusion, charge transfer, adsorption and coupling with a bulk reaction on rough electrodes. All theories are developed accounting the influence of ubiquitous uncompensated solution resistance in an electrochemical system. The random electrode surface topography governs the significant part of electrochemical response for the interfacial processes. The statistical theoretical approaches developed here provide deeper physical insights into the phenomenological intricacies involved in various complex electrochemical systems and their coupling to roughness. The statistical morphological characteristic of the electrode is incorporated through the power-spectrum of roughness. The theoretical modeling applied here uses the second order perturbations in roughness profile to obtain admittance response of planar and rough electrode. Derived equations unravel the different frequency regimes, the underlying governing phenomena, the associated phenomenological time and length scales. The interplay of phenomenological lengths, viz. dynamic diffusion length, ohmic-diffusion, kinetic-diffusion, adsorption-diffusion coupling lengths and morphological lengths determines the electrode response. Equations for the admittance voltammetry and electrochemical impedance spectroscopy for the multiscale finite fractal roughness are used for the detailed analysis. For the finite fractal model, statistical morphological parameters of roughness, viz., fractal dimension, topothesy length and lower cut-off length significantly influence the admittance response. The contribution of adsorption, charge transfer kinetics and uncompensated solution resistance is also observed in the electrochemical responses. The experimental validity of theoretical result for EE scheme has been carried for ethyl viologen dibromide system on rough Pt-electrode. The theoretical predictions are in accord with the experimental observations. Finally, our current methodology for admittance voltammetry has the dual advantage of impedance as well as of voltammetry.

*Contents*

1. Introduction 2. Theory for admittance voltammetry of reversible two step electron transfer process with DC bias at rough and fractal electrodes 3. Theory for admittance voltammetry in presence of uncompensated solution resistance for E and EE processes at rough at rough electrode 4. Theory for admittance voltammetry of

EC' reaction in presence of uncompensated solution resistance at rough and fractal electrode 5. Theory for DC biased admittance of adsorption coupled to quasireversible charge transfer with uncompensated solution resistance at rough electrode 6. Summary and future perspectives.

30. MITTAL (Ayushi)
**Fabrication of Lipase Mediated Nanocarriers for Biomedical Applications & Synthesis of Graphene Based Heterogeneous Catalyst for Organic Transformations.**
Supervisor : Prof. Sunil K. Sharma
<u>Th 25559</u>

*Abstract*
*(Not Verified)*

Molecular self-assembly, the spontaneous process of forming ordered aggregates without external intervention is gaining attention by researchers from different disciplines due to its wide-spread applications. The phenomenon is derived mostly by various non-covalent interactions such as hydrophobic, ionic, π- π stacking and electrostatic interaction adopting minimal Gibbs free energy and thermodynamic stability. The natural self-assembly phenomenon for example polypeptide chains folding into proteins or conformational changes of nucleic acids into their different functional forms etc. have inspired the scientific community to mimic the process using newly designed molecules. Self-assembly of amphiphilic macromolecules provide a unique and newer opportunity for designing novel material for advanced applications in biomedicine and bio-nanotechnology. Among the diverse and various promising applications of amphiphilic macromolecules, the area of drug delivery is challenging because of the limited aqueous-solubility and short circulation half life of most clinically used drugs. Carrier mediated drug delivery not only can maximize the bioavailability but also allow targeting the active site in the body while minimizing the side effects. Amphilphiles can self-assemble into a variety of nano- and microscale structures in the aqueous medium, where the majorly known 3-D structures include vesicles, micelles and molecular gels. However, our interest is to explore the use of different competing moieties in amphiphilic systems which can improve the aqueous-solubility for hydrophobic guests and make them suitable candidates for drug delivery. In this regard, Polyethyleneglycol (PEG) and an oligomer of glycerol *i.e.* triglycerol, diglycerol have been suitably modified to develop the desired novel nanocarriers. PEG is considered due to its specific desirable properties such as non-toxicity, chemical stability, aqueous solubility, biocompatibility, less interaction with blood component and tendency to resist protein adsorption.

*Contents*

1. Febrication of oligo-glycerol based hydrolase responsive amphiphilic nanocarriers 2. Fabrication of diglycerol based gemini amphiphiles for transdermal drug delivery 3. Synthesis of $C_3$-symmetric star shaped amphiphiles for drug delivery applications Graphene oxide based copper complex: a new heterogeneous catalyst for *N*-Arylation and C-H activation. Summary, Papers published.

31. MUNJAL (Mehak)
**Synthesis and Characterization of Anode and Cathode Nanocatalyst for the Production of Bioelectricity in Microbial Fuel Cell.**
Supervisor : Prof. Raj Kishore Sharma and Dr. Meenakshi Sharma
<u>Th 25030</u>

*Abstract*
*(Not Verified)*

The main objective of this thesis is to synthesize (a) low cost anode that allows effective bio film formation and a rapid extracellular electron transfer; (b) an effective cathode catalyst with enhanced kinetics of oxygen reduction reaction. This thesis described a comprehensive and a comparative study for the study of the surface morphological and electrochemical properties of the spinel metal oxide as the anode and cathode electrodes of the MFCs. Spinel type oxides offers a high electrochemical capacitance, multiple redox centers, high electrical conductivity and bio-compatibility. In addition to this, the long term stability while maintaining the structural integrity. Chapter 1 gives the brief introduction to the Microbial fuel cell and its components. Chapter 2 covers the structural and electrochemical techniques used to characterize the different spinel oxides and their composites. Chapter 3 highlights a facile strategy to fabricate anode based on Cobalt Ferrite (CF) and deposited over graphite sheet to envision a cost-effective MFC anode. Next, in chapter 4, we reported the synthesis of Cobalt ferrite with polyaniline (CF/PANI) and demonstrated it as a efficient anode material for the high performance MFC. Chapter 5 highlighted a facile strategy to synthesize nitrogen doped Nickel cobalt oxide nanoflowers by hydrothermal method. It is concluded that ease of preparation, low cost, high electrochemical activity and biocompatibility makes the spinel oxide, an efficient bifunctional electrode material for Microbial Fuel cells. Additionally, the aim of this research work, set out in the beginning of the thesis has been addressed. The results presented in the thesis suggest that spinel based oxide and their composite can be effectively used as an anode and cathode electrocatalysts for the high performance Microbial fuel cells.

*Contents*

1. An overview on microbial fuel cells 2.Characterization techniques and evaluation parameters 3. An insight of bio clectricity production in mediator less microbial fuel cell using mesoporous cobalt ferrite anode 4. Cobalt Ferrite/PANI nanocomposite as an efficient anode catalyst in microbial fuel cell 5. Nitrogen doped nickel cobalt oxide nanoflower: an efficient cathode catalyst for microbial fuel cell 6. Conclusions and future perspectives. List of publications.

32. NAGPAL (Mudita)
**Synthesis, Characterization and Applications of Porous Calcium and Magnesium based Adsorbents for Removal of Toxic Organic Pollutants.**
Supervisor : Prof. Rita Kakkar
Th 25056

*Abstract*
*(Verified)*

With the increasing rate of urbanization and the consequent increase of wastewater generation, the serious threat to human life, flora and fauna is also increasing. Wastewater contains several hazardous organic pollutants like organic dyes, pesticides, pharmaceutical compounds, disinfection by-products and various industrial chemicals. These organic pollutants possess stable chemical structures and are difficult to degrade. Adsorption has emerged as an efficient method for the removal of pollutants owing to its simplicity, effectiveness, flexibility, good regeneration and insensitivity to toxic pollutants. The research work in this thesis is aimed to study the synthesis, characterization and applications of porous calcium and magnesium based adsorbents for efficient removal of toxic organic pollutants

from wastewaters. The low toxicity, basic nature, high surface area, porosity and large number of active sites are some of the important features which render calcium and magnesium based adsorbents advantageous over other adsorbents. In the first study (Chapter 3), hierarchically porous calcium oxide (Hr-CaO) has been synthesized via an environment friendly precipitation and calcination method. Hr-CaO has been used for the adsorption of organophosphate pesticide, phosmet. FTIR, XRD, DFT and LCMS studies confirmed exothermic destructive adsorption of phosmet. The next study (Chapter 4), focusses on the competitive adsorption of Congo red and phosmet on hierarchically porous Ca-Mg mixed oxide (Hr-CaO.MgO). Wastewater from industries generally contains mixtures of pollutants. Therefore, the selectivity of an adsorbent for specific types of pollutants is an important factor. Mesoporous magnesium oxide-graphene oxide composite has been synthesized using a post immobilization method in the next study (Chapter 5). The composite exhibits a highly selective adsorption of anionic dyes from binary mixtures of cationic and anionic dyes. The last study focusses on the low cost synthesis of SDBS modified vaterite microspheres (Hr-SMV) and the application of Hr-SMV for the selective adsorption and separation of hazardous cationic dyes.

*Contents*

1. Use of metal oxide for the adsorptive removal of toxic organic pollutants 2.Experimental and computational techniques 3. The adsorptive degradation of phosmet using hierarchically porous calcium oxide: an experimental and theoretical study4. The adsorptive removal of congo reg in the presence of an organophosphate pesticide using hierarchically porous Ca-Mg missed oxide (Hr-CaO.MgO) 7. Conclusions and perspectives. Bibliography

33. NEHA
**Generalized Theory for the Dynamics of Multiscale Gaussian Polymeric Structure.**
Supervisor : Prof. Rama Kant
Th 25082

*Abstract*
*(Not Verified)*

The work in the thesis focuses on the static and dynamics of homo- and heteropolymeric structures. For the heteropolymers, we developed a theoretical multiscale generalized Gaussian structure (mGGS) formalism. The multiscale nature is described as a variable size of monomers connected to each other through harmonic springs with different spring constants. This formalism allows studying various static and dynamic properties like the mean displacement of a specified monomer under external (unit step) forces, dynamic moduli, intrinsic viscosity, static structure factor, etc. The heteropolymeric structures which we are studied in this thesis are polymer grafted nanoparticles, dendrimer grafted nanoparticles, linear block copolymers, miktoarm. Whereas the dynamics of star and dendrimer homopolymeric structures studied under the influence of layered random flow through Matheron-de Marsily flow model. Three dynamic properties of polymer grafted nanoparticles are analyzed in this thesis, viz. the mean displacement of a specified monomer of the polymer chain and its time evolution under external (unit step) forces, dynamic moduli, intrinsic viscosity. The viscoelastic properties, viz. the dynamic moduli, intrinsic viscosity and static structure factor of dendrimer grafted nanoparticles are analyzed. The influence of nanoparticles in dendrimer structure is reflected in different frequency regimes of the dynamic moduli. The static and dynamic properties of linear block copolymer are analyzed in dilute solution. The dynamic moduli of block copolymer manifested through different frequency regimes.

The strong effect of heterogeneity is observed in Kratky plot of the static structure factor. The static and dynamic properties of miktoarm is also analyzed through this multiscale approach. The effect of monomeric properties in miktoarm polymers is observed in the dynamic moduli and the Kratky plot of the static structure factor. We developed a theory with inclusion of ubiquitous excluded volume interactions on average square displacement (ASD) of the center of mass in layered random flow.

*Contents*

1. Introduction to the theoretical aspect of polymer dynamics 2. Theory for the dynamics of polymer grafted nanoparticle in solution 3. Static factor and viscoelastic properties of dendrimer grafted nanoparticles in solution 4. Theory for the dynamics of linear block copolymer in solution: viscoelastic properties and static structure factor 5. Theory for the static and dynamics of miktoarm in solution 6. Influence of excluded volume interactions on the dynamics of dendrimer and polymers in layered random flow 7. Summary and future perspectives.

34. PANDEY (Shetank Shashi)
**GIS based Temporal, Bi-variate, Multi-variate and Toxicity Analysis of Groundwater Uranium with Associated Water Parameters in the Central Ganga-Yamuna basin of India.**
Supervisor : Prof. Balaram Pani
Th 25560

*Abstract*
*(Not Verified)*

The study deals with the determination of uranium and associated water-parameters in groundwater samples of the central Ganga-Yamuna basin of India, by using LED-fluorimeter, Moran'I-correlation, Pearson-correlation, PCA and chemical toxicity analysis. In the pre-monsoon season, uranium mean values were observed at 4.95µg/L, 4.81µg/L, and 11.79µg/L in upper, middle and lower regions, respectively. However, in the post-monsoon season, uranium mean values were observed at 3.34µg/L, 5.65µg/L, and 14.04µg/L in the upper, middle and lower regions, respectively. The groundwater of all three regions was determined to be neutral to alkaline in nature and it was observed that the mean pH was increased after the monsoon. The most abundant uranium species found was Ca2UO2(CO3)3.. The positive-relationship between TDS and uranium in groundwater reflects the impact of weathering. In most cases, uranium has a positive-relation with total alkalinity, indicating the possibility of the formation of uranyl carbonates/bicarbonates complexes that do not adsorb to minerals and metal oxides in the soil and keep uranium in a soluble form in groundwater. Uranium was also shown to be positively-related to total hardness in the regions, indicating that calcium and magnesium ions influence uranium-speciation. The PCA revealed that groundwater of the study region was affected by agricultural sources, weathering, dissolution of minerals, sewage intrusion, evaporation and water recharge processes. In both the seasons of the upper region, possible sources of uranium concentration in groundwater were geogenic. In the post-monsoon season of the middle region, uranium has strong loading with phosphates which indicates the contribution of uranium to the groundwater from the anthropogenic activity. Overall, the main source of uranium in the study area is geogenic in nature but the various anthropogenic activities affect its mobility. The chemical and radiological risks due to uranium intake for adults and children lie within the safe limits of 4.53µg/kg/day and 1.67×10-4, respectively.

*Contents*

1. Introduction 2. Review of literature 3. Material and methods 4. Results and discussion 5. Conclusion. References, List of publications.

35. PATANJALI (Pooja)
**Preparation, Characterization and Application of Bentonite Based Adsorbents for Cationic Dye Removal.**
Supervisor : Dr. Rajeev Singh
Th 25046

*Abstract*
*(Not Verified)*

The thesis entitled “Preparation, Characterization and Application of Bentonite Based Adsorbents for Cationic Dye Removal” presents the synthesis of bentonite based adsorbents and their application for cationic dye removal form aqueous solutions. The subject matter in the thesis is divided into five chapters. Chapter I deals with the general introduction including classification of clays and various clay modification techniques. It also covers the relevant literature for surface modification and formation of bentonite composites which serve as a background for subsequent chapters. Chapter II describes the synthesis of surfactant modified bentonite using two cationic surfactants: Cetyltrimethylammonium bromide (CTAB) and Trioctylmethylammonium chloride (TOMAC) and their application for removal of cationic dyes (Methylene blue, Crystal violet and Rhodamine B) from aqueous solutions. Chapter III deals with the synthesis of silane grafted bentonite using 3-aminopropyltriethoxysilane (APTES) and 3-mercaptopropyltrimethoxysilane (MPTMS) and their application for cationic dye removal from aqueous solutions. Chapter IV describes the synthesis of bentonite-alginate beads (BAB) and bentonite-alginate-double walled carbon nanotube beads (BACB) for cationic dye removal from aqueous solutions. Chapter V deals with the synthesis of bentonite based hydrogel composites and their application for cationic dye removal from aqueous solutions. Chapter II, III IV and V also include the characterization of synthesized adsorbents using X-ray diffraction (XRD), Fourier transformed infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), Thermal Gravimetric Analysis (TGA) and Brunauer-Emmett-Teller (BET) surface area analysis. During the adsorption experiments, effects of different physicochemical variables like pH, adsorbent dose, contact time and initial dye concentration on adsorption performance were also evaluated. The data obtained from the series of adsorption experiments was fitted with various kinetic models [Pseudo-first-order (PFO), Pseudo-second-order (PSO), Elovich, Intra-particle diffusion (IPD) models] and adsorption isotherms (Langmuir, Freundlich, Temkin isotherm). Finally, the adsorbents were evaluated for their reusability potential through repeated cycles of adsorption and desorption.

*Contents*

1. General Introduction 2. Surfactant modified bentonite for removal of cationic dyes 3. Silane frafted bentonite for removal of cationic dyes from aqueous solutions 4.Calcium alginate-bentonite composites for removal of cationic dyes 5. Bentonite based hydrogel composites for dye removal. Summary and Publications.

36. RASHMI
**Design and Synthesis of Non-ionic Amphiphilic Architectures as Nano-transporters.**
Supervisor : Prof. Sunil K. Sharma
Th 25080

*Abstract*
*(Verified)*

The thesis entitled: “Design and Synthesis of Non-ionic Amphiphilic Architectures as Nano-transporters' consist of variety of non-ionic amphiphilic architecture that include the synthesis of non-ionic bolaamphiphiles and study of their self-assembly and transport behavior for drug delivery applications, PEG-Oligoglycerol conjugated nano-carriers for transdermal delivery, stimuli-responsive, non-ionic gemini amphiphiles for drug delivery applications and supramolecular engineering of alkylated, fluoroalkylated and mixed amphiphiles. All the sysnthesised amphiphiles were well characterized and their physiochemical studies were performed. They all found to be potent molecules for biomedical applications.

*Contents*

1. Synthesis of non-ionic bolaamphiphiles and study of their self-assembly and transport behavior for drug delivery applications 2. PEG-oligoglycerol conjugated nano-carriers for transdermal delivery 3. Stimuli-responsive, non-ionic geminiamphiphiles for drug delivery applications 4. Supramolecular enfineering of alkylated, fluoroalkylated and mixed amaphiphiles. Summary and papers published.

37. RAWAT (Manish)
**Design and Assembly of Metal Based Catalytic System for Green and Sustainable Synthesis of Biologically Active Heterocycles.**
Supervisor : Prof. Diwan S. Rawat
Th 25047

*Abstract*
*(Not Verified)*

In chapter 1a, Synthesis of biologically active fused imidazo[1,2-a]pyrimidines were achieved via A3 coupling of 2-aminobenzimidazole, aldehyde and terminal alkyne, followed by 6-endo-dig cyclization using copper oxide nanoparticles under solvent free condition is described. In chapter 1b, A novel CuO@NiO nanocatalyst was prepared by simple calcination of mixture of malachite as sustainable copper source and nickel oxalate. The obtained CuO@NiO nanocatalyst was found to be an efficient heterogeneous catalyst for the synthesis of indenoisoquinolines from 2-iodobenzamide and 1,3-indanedione using ethylene glycol as a green solvent. In chapter 2a, A green approach for the synthesis of 2-aminonicotinonitriles from oxime acetate as enamine precursor, aldehyde and malononitrile under neat condition without the use of additive in presence of CuI@Al2O3 nanocatalyst is reported. In chapter 2b, Cu2O nanoparticles were successfully embedded over marigold hollow alumina microspheres (MHAM). Cu2O@MHAM nanocatalyst exhibited excellent catalytic potential towards synthesis of isoquinolone from 2-bromobenzonitrile and acetophenone under sustainable reaction condition.In chapter 3a, We developed a facile approach for the preparation of magnetically recoverable cuprous oxide supported over a poly(m-pheneylenediamine) coated magnetic nanoparticle (Fe3O4@PmPDs) and their catalytic efficiency for the green synthesis of 5-phenyl-[1,2,3]triazolo[1,5-c]quinazolines from (E)-1-bromo-2-(2-nitrovinyl)benzenes, aldehydes, and sodium azide under mild reaction condition. In chapter 3b, We developed a CuO@MgO catalysed synthesis of isocoumarins by reaction between 2-iodobenzoic acids and terminal alkynes without any base or additive in polyethylene glycol solvent. In chapter 4, A highly regioselective [Cp*Co(CO)I2] catalyzed addition of 1,3-diketones to terminal alkynes at room temperature have been achieved using Cu(OTf)2 as a co-catalyst. Reaction of 1,3-diketones having substitution at active

methylene carbon with phenyl acetylenes having electron withdrawing group or bulky group results in the formation of 2-alkenylated 1,3-dicarbonyl product, but phenyl acetylenes with electron donating group led to the formation of tetrahydronaphthalene and terphenyl.

*Contents*

1a. Synthesis of copper oxide nanoparticles and its application in the synthesis of imidazo[1,2-a]pyrimidine derivatives, their optical properties and selective fluorescent sensor towards zinc ion 1b. A green and sustainable approach for the construction of CUO@NiO nanocomposites and its application in the synthesis of biologically active indenoisoquinoline derivatives 2a. Preparation of CuI@$Al_2O_3$ nanocomposites for the synthesis of 2-aminonicotinonitrile derivatives under solvent free condition 2b. Fabrication of $Cu_2O$ devorated marigold hollow alumina microspheres (MHAM) nanoparticles and their role as robust and efficient catalyst for the synthesis of isoquinolone 3a. Design and proparation of magnetically separable $Fe_3O_4$@poly)m-phenylenediamine)@$Cu_2O$ nanocomposites for the synthesis of 5-phenyl-[1,2,3]triazolo[1,5-c]quinazolines 3b. Development of mesoporous copper-magnesium oxide nanohybrids and its application in the synthesis of 3-substituted isocoumarins from 2-iodobenzoic acid and terminal alkyne under green conditions 4. [Cp*Co(CO)I2] catalysed C-C bond formation and [2+2+2] annulation of 1,3-dicarbonyls to terminal acetylenes. Summary, List of publications, Honors and awards, Conferences, seminar and workshops.

38. RAWAT (Srishti)

**Design, Synthesis and Characterization of Biologically Active Heterocyclic Compounds.**

Supervisor : Prof. Diwan S. Rawat

Th 25063

*Abstract*
*(Not Verified)*

Chapter 1 deals with QcrB, a subunit of cytochrome bcc which is present in respiratory chain of mycobacterium is the target of Q203 (anti-tb agent) currently in phase II clinical trial. As expected, its inhibition leads to depletion in ATP levels, compromising the cell function. We described about structure, functions and an overview of chemical classes of all inhibitors of QcrB known which would help in the development of new chemical entities. Chapter 2 deals with design and synthesis of indole-5-acetamides and benzoxazole-triazole derivatives in multi-step process using the hybridization approach. A variety of derivatives were synthesized by varying 1st and 5th position of indoles in indole-5-acetamides while in benzoxazole-triazole hybrids variation at 2nd and 5th position of benzoxazoles were done. Derivatives were characterized and in vitro antitubercular activity of both series of compounds are discussed. Chapter 3a deals with design, synthesis and screening for initial one-dose anticancer activity. Compounds shows 60-80% growth percent for UO-31 renal cancer cell line and follow in-silico pharmacokinetic parameters i.e. ADME and Lipinski's rule of five. Chapter 3b deals with studies of aminoquinoline-pyrimidine (AQ-PY) hybrids attached to piperazine and alkyl linker. Mechanistic heme binding studies confirmed that compounds binds to heme slightly more effective than CQ and confirms it to be most probable target. While the molecular docking shows moderate binding with mutant Pf-DHFR-TS to validate Pf-DHFR enzyme as other target for hybrids. Chapter 4a deals with catalytic potential of CuO@Fe2O3 MNPs catalyst for C1-alkynylation of THIQ via A3 coupling and its decarboxylative strategies. Catalyst was found to be robust, magnetically recoverable, recycled and follow green chemistry metrics. In Chapter 4b, metal free one pot C1-indolylation and N-alkylation of THIQ is reported using recyclable PEG600 solvent. A wide range of derivatives were synthesized by varying aldehyde and indole derivatives and follows green chemistry metrics.

*Contents*

39. KM SHALLY
**Multifunctional 1,2,3,4-Tetrahydroquinolines, Arenes and Furans : Synthesis and Photophysical Properties.**
Supervisor : Prof. Ramendra Pratap
Th 25069

*Abstract*
*(Not Verified)*

The thesis entitled "Multifunctional 1,2,3,4-Tetrahydroquinolines, Arenes and Furans: Synthesis and Photophysical Properties" is submitted to University of Delhi. It includes design, synthesis and structural elucidation of multifunctional 1,2,3,4-tetrahydroquinolines, arenes and furans and mechanistic investigation of the reactions involved in their synthesis. The synthesized molecules were used for further modification. These reported compounds were synthesized by using suitably functionalized 2H-pyran-2-ones, 2-oxobenzo[h]chromones and ketendithioacetals as precursors. The whole work presented in this thesis has been divided into four chapters. In the chapter 1, we have explored the application of 2H-pyran-2-ones and N-boc-3-piperidone for the synthesis of functionalized 1,2,3,4-tetrahydroquinolines and quinolines. We have investigated the mechanistic approach for their synthesis. We have studied photophysical properties of the synthesized compounds. Two compounds namely 6-orpholino-8-(thiophen-2-yl)-1,2,3,4-tetrahydroquinoline-5-carbonitrile and 6-(methylthio)-8-(thiophen-2-yl)-1,2,3,4-tetrahydroquinoline-5-carbonitrile act as selective chemosensors for palladium ion. In the chapter 2, we have reported the synthesis of arylated anilines and aminated dihydrophenanthrenes through arylacetonitriles mediated ring transformation of 2H-pyran-2-ones/2-oxo-benzo[h]chromenes and their photophysical studies has been carried out. In addition, the synthesized compound 2''-bromo-[1,1':2',1''-teraryl]-3'-amines undergoes cyclization to afford carbazole in excellent yield. In the chapter 3, we have reported the synthesis of biaryls and teraryls from newly developed suitably functionalized ketenedithioacetals and study of their photophysical properties was performed. We have also investigated the mechanistic approach for the synthesis of biaryls and teraryls. In the chapter 4, we have reported the synthesis of multifunctional furans and pentasubstituted benzenes form ketenedithioacetals under basic condition. We have studied the role of steric factor in both substrates (ketenedithioacetals and nucleophiles) on reactivity. We observed that substitution pattern in substrates play a major role in tuning the reactivity and selective formation of furans or biaryls. We have also investigated the mechanistic pathway for their synthesis.

*Contents*

1. 1,2,3,4-Tetrahydroquinolines and quinolones: synthesis photophysical properties and $Pd^{2+}$ ion recognition 2. Synthesis of arylated anilines and aminated 9,10-dihydro-phenanthrenes through arylacetonitriles mediated ring transformation of 2*H*-pyran-2-ones/2-oxobenzo[*h*] chromens and their photophysical studies 3. Synthesis of biaryls and teraryls from suitably functionalized ketenedithioacetals and their study of photophysical properties 4. Substrate directed synthesis furans and pentasubstituted benzenes. List of publications, Conferences attended.

40. SHALU

**Investigation of Few Mixed Metal Oxides with Interesting Optical, Magnetic, Catalytic and Ion-Exchange Properties.**

Supervisor: Prof. Sitaraman Uma

Th 25038

*Abstract*

*(Not Verified)*

The present thesis is aimed on the exploration of some aspects of oxides and divided into four chapters. The importance of research in the area of mixed metal oxides is highted by taking suitable examples and introduced in chapter one. The relevance of structure-property correlation in oxides is also elaborated with appropriate examples. Chapter two is fully devoted for the work carried out on layered oxide compounds. It deals with the synthesis of new layered perovskite oxides (i) utilizing a combination of topochemical reactions and (ii) adopting exploratory synthesis. Protonated oxides, H2[Sr2Nb2MO9.5] (M = Al, Ga) and H2[Sr2Nb2ZrO10] related to the Ruddlesden-Popper (RP) family of layered perovskite oxides have been synthesized using Bi2Sr2Nb2MO11.5 (M = Al, Ga) and Bi2Sr2Nb2ZrO12 Aurivillius (AV) phases. The solid state synthesis of new Dion-Jacobson (n = 3) layered perovskites, A'Cd2Nb3O10 (A' = Rb, Cs) was also successful. The mobilities of these interlayer ions in layered oxides have been confirmed by ionic conductivity measurements. The exploration of metal sulfide to metal oxide conversion has been described in chapter three. CuSbS2 system was stabilized by the co-thermal decompositions of the equimolar concentrations of thiourea complexes ([Cu(tu)3]Cl and [Sb(tu)2]Cl3) in ethylene glycol and ethanolamine sulfides. Additionally, we explored the possibility of conversion of chalcostibite (CuSbS2) to sulfur-doped trirutile-structured CuSb2O6. All of these samples were examined towards the photodegradation of carcinogenic rhodamine 6G (Rh 6G). The results of study of converting the mineral beyerite to mesoporous CaBi2O4 has been discussed in chapter four. Reduction of harmful 4-nitrophenol and carcinogenic Cr(VI) was catalyzed by CaBi2O4 efficiently and their kinetics study has also been examined. The overall conclusions emerged from the present set of investigations are summarized at the end. Additionally, its implications towards either practical application or to carry out further studies for any futuristic applications to mankind are elaborated.

*Contents*

1. Introduction 2. Novel layered perovskite oxides 2.1 Soft chemical synthesis of $Al^{3+}$, $Ga^{3+}$, and $Zr^{4+}$ containing layered perovskite oxides 2.2 Dion-jacobson layered perovskites in non-centrosymmetric space group 3. Exploring metal 3.1 Wet-chemical synthesis of $CuSbS_2$, $Cu_3SbS_3$, and bismuth substituted $Cu_3$ $SbS_3$3.2 Exploring the conversion of $CuSbS_2$ to S-doped $CuSb_2O_6$ 4. Conversion of beyerite

into mesoporous $CaBi_2O_4$. Overall summary and future directions, List of publications.

41. SHAW (Ranjay)
**Synthesis of functionalized 2H-Pyran-2-ones, Axoles, Fluorenones and Benzenes from Ketene Dithioacetals.**
Supervisor : Dr. Ramendra Pratap
Th 25062

*Contents*

1. C-C bond formation by C-S bond cleavage for the synthesis of diarylated 2H-pyran-2-ones, chalcones and azoles 2. Chemoselective synthesis and fused ketene dithioacetals and their anti-HIV-1 activity 3. Synthesis of allyl arenes ring transformation of 2*H*-pran-2-ones by 5-hexene-2-one and their synthetic applications 4. Synthesis of 3-aryl-5-thiomethyl-phenols from ketene dithioacetals through base mediated [3+3] cycloaromatiosation. List of publicatons.

42. SHIV KUMAR
**Transition-Metal-Free Approaches for the Construction of *N*-Heterocycles and Deuteration of Terminal Alkynes.**
Supervisor: Prof. Akhilesh Kumar Verma
Th 25037

*Abstract*
*(Not Verified)*

A metal-free tandem reaction is demonstrated to be the specific tool for the variety of synthetic applications. Several reports are available in the literature showing the importance of chlorinated heterocyclic compounds. The intramolecular and intermolecular cyclization of chlorinated heterocyclic and quinoline core have certain drawbacks such as longer reaction time, limited substrate scope, expensive metal catalysts, availability of starting materials, and requirement of multi-step procedures. For the synthesis of a long range of nitrogen, oxygen, and sulfur (N/O/S) containing heterocycles, Ortho-alkynylaldehydes and primary amines are among the most widely used precursors. 1,2-Dihydroisoquinoline core nucleus is found in a range of natural products and pharmaceutical compounds. Metal-free electrophilic iodocyclization without oxidizing alcohol in the reaction is proving to be particularly useful in a wide variety of synthetic processes. A lot of literature is available explaining the importance of esters and bio-active dihydrofuran/pyran with deuterium labeling studies. Various research groups showed the synthesis of esters and bio-active dihydrofuran/pyran, deuterium labeling studies with certain drawbacks such as availability of starting materials, the limited scope of use, and expensive metal catalysts. The triazole moiety is an important organic molecule falling under the class of fused N-heterocyclic that has been explored for the identification/discovery of bioactive agents and drugs heterocycles. It has stimulated a great deal of research into the construction of substituted 1,2,3-triazole. The rapid and experimentally simple construction of 1,2,3-triazole molecules under mild reaction conditions is of high demand, [3+2] cycloaddition reaction is one of the most common methods that has been utilized for the synthesis of a variety of bioactive antibiotics, antimicrobial resistance active compounds. Several methods are present in the literature for the preparation of substituted 1,2,3- triazole compounds with certain drawbacks as a limited substrate scope, multi-step procedures, unavailability of starting materials, expensive metal catalysts. Terminal alkynes and DMSO-d6 one-pot reactions have proven to be a useful tool for synthetic processes.

A literature survey revealed that DMSO-d6 was used as a source for the deuteration of terminal alkyne and has not been extensively studied. Thus, new efficient approaches for the synthesis of deuteration of aromatic and aliphatic terminal alkynes are in high demand.

*Contents*

1. Dual function of carbon tetrachloride: synthesis of chlorinated heterocycles 2. Chemoselective oxidative esterification and iodocyclization of Hydroxyalkynyl aldehydes 3. Base-mediated three-component route to 1,2,3-triazole-4-carboxylate using aldehyde, amine, and diazoacetate 4. Super-base catalyzed mono-selective deuteration of alkynes. Summary of the work, Copies of the publications.

43. SHRIVASTAVA (Vipul)
**Magnetic and Catalytic Properties of Few Ternary Vanadium-Containing Oxides, Substituted $PrAlO_3$, and γ-$Bi_2O_3$ Systems.**
Supervisor : Prof. Rajamani Nagarajan
Th 25028

*Abstract*
*(Not Verified)*

The multifunctional aspects of mixed-metal oxides are discussed by correlating it with different structures adopted in a few vanadium-containing ternary oxides (spinels, and pyrovanadates), different polymorphs of Bi2O3, and single perovskites.MgV2O4, and ZnV2O4 were synthesized by epoxide mediated sol-gel route. Partial substitution of magnetic ions (Cr3+, and Fe3+), and non-magnetic ion (In3+) at the vanadium site are performed for the first time. Paramagnetic character of MgV2O4 and ZnV2O4 changed to antiferromagnetic and ferromagnetic/ ferrimagnetic character on substitution with chromium and iron ions, respectively as evident from its temperature-dependent magnetic measurements. ZnVInO4 showed excellent photocatalytic activity in the degradation of Rh-6G dye solution in presence of UV-visible light source. a-Zn2V2O7 and Zn3V2O8 were synthesized by a simple facile co-precipitation route by using NaOH as precipitating agent. Further, conversion of benzyl alcohol to benzaldehyde and degradation of crystal violet (CV) dye solution were catalyzed by these samples under UV-visible light irradiation.PrAlO3 was synthesized by auto combustion, and sol-gel techniques. Upto 20 mol % of bismuth was substituted in place of praseodymium by retaining rhombohedral symmetry. Substitution of bismuth brought reduction in optical band gap, and improvement in catalytic (conversion of p-nitrophenol to p-aminophenol), and photocatalytic (degradation of CV dye) activities. Substitution of 70 % iron at praseodymium site was achieved (upto 40 mol%, rhombohedral symmetry, upto 70 mol %, orthorhombic symmetry). The presence of Fe2+/Fe3+ coupled with Pr3+/4+ manifested in multiferroic properties and higher catalytic efficiency.

*Contents*

1. Introduction 2. Work related to vanadium-containing ternary oxides 3. Effects of including $In^{3+}$ions on the structure and properties of γ-$Bi_2O_3$4.Consequences of cationic substitutions in $PrAlO_3$ perovskite. Conclusions and future directions. List of publications.

44. SHARMA (Aditi)

**Unlocking High Catalytic Performance of Nanostructured Graphene Oxide and Cobalt Oxide based Materials for Amidation, C-H Activation, Cyclization and Condensation Reactions.**

Supervisor : Prof. R. K. Sharma

Th 25052

*Abstract*

*(Not Verified)*

The present work has been divided into six chapters. A brief discussion of each of these is given below: Chapter 1 deals with the general introduction of nanostructured graphene oxide and cobalt oxide based material and their application in the field of catalysis. Further, succinct overview of the synthetic procedures, functionalization strategies and characterization techniques of the developed nanocomposites has been discussed. Chapter 2 provides information about the various physico-chemical techniques that have been employed for the complete characterization of organic-inorganic hybrid nanomaterials and synthesized products. In Chapter 3, we present the first report of an atom economical and environmentally benign amidation of unactivated esters wherein a novel and highly versatile graphene oxide based cobalt nanocatalytic system has been effectively exploited for the synthesis of pharmaceutically significant amide derivatives under neutral reaction conditions. In Chapter 4, pharmaceutically and biologically important compounds containing imidazo[1,5-a]pyridine nuclei have been synthesized via transannulation of N-heteroaryl aldehydes or ketones with alkylamines using a graphene oxide-supported copper catalyst. In chapter 5, we report magnetically retrievable graphene oxide based copper nanocatalytic system that has been effectively exploited for obtaining a series of pharmaceutically and biologically active benzoxazole scaffolds. In chapter 6 we disclose the first report to study the catalytic activity of nonagglomerated and redispersible Co3O4 nanocages decorated with nickel nanoparticles for the synthesis of pharmaceutically and biologically important compounds containing N-heterocyclic quinoxaline nuclei using α-dicarbonyls and 1,2-diamines as precursor reagents. The structure of all synthesized nanocatalysts was confirmed by various microscopic and spectroscopic techniques such as transmission electron microscopy, scanning electron microscopy, X-ray photoelectron spectroscopy, X-ray diffraction, fourier transform infrared spectroscopy, energy dispersive X-ray fluorescence spectroscopy, atomic absorption spectroscopy and elemental analysis.

*Contents*

1. Introduction 2. Theory and principles of characterization techniques 3. Unprecedented ester-amide exchange reaction using highly versatile two-dimensional graphene oxide supported base metal nanocatalyst 4. Design and exploration of catalytic activity of two-dimensional surface-engineered graphene oxide nanosheets in the transannulation of n-heterocyclic aldehydes or ketones with alkylamines 5. A simple and straightforward strategy for expedient access to benzosazoles using chemically engineered 2D magnetic graphene oxide nanosheets as an eco-compatible catalyst 6. Finely tuned catalytic $Co_3O_4$ nanocages decorated with base metal nanoparticles: A highly integrated and sustainable platform for the synthesis of pharmaceutically active quinoxaline derivatives. Summary, List of publications, List of conferences/seminars/symposia participated.

45. SHARMA (Anu)
**Development of Multifunctional Drug-Loaded Metal-Organic Frameworks for Multiple Pathological Conditions.**
Supervisor : Dr. Rakesh Kumar Sharma
Th 25079

*Abstract*
*(Verified)*

The first chapter describes a brief introduction of the scientific literature on the topic of nanotechnology, nanoclusters, and metal-organic frameworks outlining their salient features. Special emphasis is laid on multifunctional Iron-phenanthroline nanoclusters, Zeolitic imidazolate framework and magnesium-gallate framework, and their biological applications which are the subject of this thesis. The second chapter reports the theory, principles and the details of the different experimental and characterization techniques used in the present investigation. The third chapter describes a new strategy to encapsulating the drug curcumin into the hydrophobic core of the iron-phenanthroline nanocomplex (NIP) and eventually its release is signified. We evaluated the anti-HIV effects of NCIP in vitro on cultures of HIV infected human microglia. The fourth chapter shows the novelty of NCIP formulation its use in the reduction of AD Plaque. We evaluated the anti-inflammatory effects of these Cur based nanoformulations by assessing the pro-inflammatory cytokines levels in the culture milieu. The fifth chapter reports synthesis of mesoporous zeolitic imidazole frameworks (ZIF- 8) and microencapsulation of organic UV filters octylmethoxycinnamate (OMC) and butyl-methoxydibenzoylmethane (BMDM) alone and in combination into mesoporous zeolitic imidazole frameworks (ZIF-8). Our findings suggest that zeolitic framework encapsulated sunscreens could provide prolonged UV-protection efficacy and ultra-high SPF with reduced potential for degradation, phototoxicity, and transport across the skin. The sixth chapter describes the synthesis of bioactive and microporous magnesium gallate Metal-organic Framework for the simultaneous delivery of anticancer agents (gallic acid and cannabidiol) to the cancer cells. CBD's anticancer actions target mitochondria by causing them to dysfunction and release harmful (ROS) reactive oxygen species. CBD/Mg-GA MOF has potential anti-cancer, anti-inflammatory and anti-oxidant properties. Thus, the present study demonstrates that CBD/Mg-GA MOF may be a promising therapeutic for glioblastoma. In the seventh Chapter, on the basis of the above observations the following conclusions have been made and reported.

*Contents*

46. SHARMA (Shivangi)
**Biomolecular Dynamics in Complex Environments: a Generalized Langevin Equation Approach.**
Supervisor : Prof. Prabati Biswas
Th 25051

*Abstract*
*(Verified)*

A stochastic-noise driven dynamical model is proposed to study the impact of noise/random fluctuations on biomolecular dynamics in the complex (viscoelastic) cellular environments within the framework of generalized Langevin equation (GLE). The viscoelasticity of the surrounding fluid gives rise to the long-range or power-law correlated thermal fluctuations, which imparts a retarding effect on the motion of the particle. Such thermal fluctuations result in emergence of anomalous diffusive dynamics of the system, which may be utilized to address two major concerns in the thesis as (i) to resolve the effect of complex cellular surroundings on the dynamics of hydration water around the protein surface in both absence and presence of active athermal fluctuations under different boundary conditions, and (ii) to explore the effect of viscoelasticity of the cellular environments on the conformational transitions of DNA hairpins and riboswitches. The results of the passage time analysis establish the fact that the hydration water dynamics around the protein surface exhibits a sub-diffusive dynamics when it is only driven by thermal fluctuations, while it follows either a sub- or super-diffusive dynamics with the consideration of additional active athermal fluctuations. This states that the active fluctuations are however necessary but not sufficient to promote super-diffusive motion. In addition to anomalous intracellular transport, a comparative study of the transition path time and Kramers's first passage time analysis offers an efficient approach to investigate the conformational transitions of DNA hairpins and riboswitches. Analytically obtained results illustrate the fact that the transition path times are shorter than the Kramers's time however, the former are insensitive to the details of the exact details of the transitions events, unlike Kramers's first passage times.

*Contents*

1. Introduction 2. Hydration water dynamics around a protein surface: a first passage time approach 3. Unusual dynamics of hydration water around motor proteins with long-ranged hydrodynamic Fluctuations 4. Conformational transitions of a DNA hairpin: a transition path time approach 5. Transition path time analysis of the effect of ligand binding on riboswitch folding. Bibliography.

47. SINGH (Ajay Pratap)
**Nanoarchitectures : Synthesis, Characterization and Photocatalytic Applications in Degradation of Noxious Organic Pollutants.**
Supervisor : Prof. M. Thirumal
Th 25070

*Abstract*
*(Not Verified)*

The need to save the environment is one of the primary importance, due to the increased environmental pollution. In this regard, the semiconductor photocatalysis has gained immense attention from the scientific world because of the great potential as one of clean environmental friendly strategies to resolve the environmental issues toward sustainable processes. Recent research on NaTaO3, NaNbO3 and Ta2O5 wide bandgap semiconductors have shown their potential to be ultimate alternatives for photocatalytic decomposition of organic pollutants. Wide bandgap of materials, restricted only to the UV spectrum that accounts for only 4—5 % of the total solar spectra, another discouraging issue is quick recombination rate of photogenerated electron-hole pairs which results in low quantum efficiency of photocatalytic

reactions. To overcome these issues, research activities have been increased to reinforce the photocatalytic properties by manipulating nanostructures or morphologies of NaTaO3 and NaNbO3 including, surface doping with non-metallic/metallic elements or semiconductor oxides and surface deposition of the noble metal nanoparticles. In the above-discussed strategies, particularly coupling with mid/narrow bandgap sensitizers such as CdS, Ag2S, and CuS to form the so-called composite heterostructures is one among the highly responsible strategy.We had synthesized NaTaO3, NaNbO3, Mg(OH)2, MgO, Bi2O3 and Ta2O5 nanomaterials and composite heterostructure of NaTaO3, NaNbO3 using facile surface functionalization method. The bandgap engineered composite heterostructures exhibited efficient harvesting of visible light with high photocatalytic organic dye degradation efficiency due to their wide range of light absorption and band alignment. Further, we had discussed the photodegradation mechanism of Rhodamine B dye to elucidate the efficiency enhancement of the composites. The thesis deals with the synthesis, characterization and bandgap engineering of nanomaterials with composite heterostructures formation for visible light photocatalytic applications. Some of the fabricated heterostructures exhibit excellent photocatalytic activity their efficiency, catalytic cycles are discussed in detail.

*Contents*

1. Introduction 2. Efficient charge transfer in hererostructures of CdS/NaTa$O_3$ with improved visible-light-driven photocatalytic activity 3. Synthesis of NaNb$O_3$-2D nanosheets and fabrication of Ag2O/NaNbO3 and multi-junction AgCl/Ag2O/NaNbO3 heteroarchitectures with enhanced visible light photocatalytic activity 4. Economical method to syntnesis of tantalum pentoxide nanoparticles from bare tantalum power: characterization and efficient photocatalytic performance 5. An efficient and xost effective synthesis approach for Mg(OH$)_2$, MgO nanoparticles and 2-D $Bi_2O_3$ nanodiscs. List of publications.

48. SINGH (Bhole)

**Design and Synthesis of fac-Re(CO)3 based Photo-active and Bio-active Metal Complexes.**

Supervisor : Prof. Balram Pani

Th 25026

*Abstract*
*(Not Verified)*

Metallacycles are discrete cyclic SCCs constructed by combining multi-topic/multi-dentate ligands and metal-ion precursors. Based on their shapes and size there are lots of supramolecular metallacycles such as mononuclear, dinuclear; trinuclear, tetranuclear-squares, rectangles, gondolas, bowls, calixarene, bicycles, hexanuclear, prisms, spheroids, wheels, and octa nuclear cycles have been developed. Pre-functionalized pyridazine derivatives (1-10) were synthesized by one-step methodologies which also include Inverse Electron Demand Diels-Alder reaction. The compounds were characterized by various spectroscopic techniques. The pyridazines were subjected to anti-microbial evaluations where few of the compounds showed moderate to high activity against most of the bacteria and fungi presented in this study. Later these compounds were used in the design and synthesis of functionalized metallacycles and their photophysical applications. In chapter 2 neutral phosphine oxide donor-based organometallic acyclic complexes were assembled from phosphine/ phosphine oxide, arylamino benzoquinone donor and Re2(CO)10 via a one-pot solvothermal approach. The complexes were characterized by elemental analysis, FT-IR, and NMR spectroscopic methods. The molecular structures of 1 and 2, were analyzed by single-crystal X-ray diffraction analysis. The UV-Visible absorption studies indicated that 1–3 in acetonitrile display strong visible light absorption in the range of ~350–700 nm. These fac-Re(CO)3 based acyclic complexes have a better affinity to intercalate with ct-DNA. A series of fac-Re(CO)3 based metallacycles (A-D) have been synthesized via solvothermal technique. These metallacycles were characterized by FTIR, 1H-NMR, ESI-MS and elemental analysis. Photophysical investigations revealed that all the complexes display strong visible-light absorption with absorption maxima at around 495 nm having higher molar extinction coefficient (e = 58000 M-1 cm-1). To further, enhance the photophysical properties a series of twelve metallacycles have been functionalized. From chapter II, pyridazine based multifunctional ditopic ligands have been utilized to synthesis a series of twelve functionalized metallacycles and photophysical properties has been investigated.

*Contents*

1. Introduction to the *fac*-Re(CO)$_3$ based metal complexes and their applications 2. Synthesis, crystal structures, and biological evaluation of new pyridazine derivatives 3. Self-assembly of phosphine oxide-based acyclic and monocyclic *fac*-Re(CO)$_3$complexes, their photophysical and DNA binding studies 4. Design, synthesis and self-assembly functionalization of *fac*-Re(CO)$_3$based photoactive and bioactive metallacycles. List of publications and List of conferences.

49. SINGH (Pragat)
**Synthesis and Spectroscopic Studies of Thiazole and Pyridine-Fused Porphyrins.**
Supervisor : Prof. Mahendra Nath
Th 25067

*Abstract*
*(Not Verified)*

The objective of this dissertation is to elaborate the design and synthesis of β,β'-heterocycle-fused meso-tetraarylporphyrins and their spectral investigation. The fusion of heterocyclic motifs through the β-functionalization of porphyrin generate molecules with interesting photophysical properties. Therefore, a variety of β,β'-heterocycle-fused meso-tetraarylporphyrins were constructed and some of these have demonstrated potential biological and material applications. The work presented in this dissertation is divided into four chapters. The first chapter of this thesis presents an account on the synthesis and photophysical characteristics of β,β'-fused 5,10,15,20-tetraarylporphyrin systems through peripheral modifications of meso-tetraarylporphyrins. Second chapter deals with the synthesis and spectral studies of novel β,β'-fused thiazolo[3,2-d]porphyrins. Third chapter of this thesis describes the synthesis of 2-chloro-3-formyl- and 3-formyl-pyrido[2,3-b]porphyrins through a modified Vilsmeier-Haack reaction procedure and their further functionalization by using Knoevenagel reaction. The last chapter describes a one-pot three-component reaction of 2-amino-5,10,15,20-tetraphenylporphyrin with the aromatic aldehydes and 4-hydroxycoumarin to produce a new series of β,β'coumarin-fused pyridoporphyrins. All the newly prepared β,β'-fused porphyrins have been evaluated for their photophysical characteristics using UV-Vis and emission spectroscopy. The preliminary results revealed a bathochromic shift in the electronic absorption and emission spectra of some of these molecules. Thus, the present study may prove useful for the designing of highly π-conjugated aromatic superstructures with exceptional light absorbing properties that find applications in the field of solar cells and photodynamic therapy.

*Contents*

1. An account on the synthesis and photophysical properties of β,β'-fused *meso*-tetraarylporphyrins 2. Synthesis and spectroscopic properties of β-thiazole-fused 5,10,15,20-tetraarylporphyrins 3. Synthesis of Pyrido[2,3-b]prophyrins under modified vilsmeier-haack conditions and study of their photophysical properties 4. Synthesis, characterization and optical properties of coumarin-fused pyridoporphyrins. Summary and Publications.

50. SINGH (Preeti)
**Design, Synthesis, Characterization and Antimalarial Activity of Newer Tetraoxane Analogs.**
Supervisor : Prof. Satish K. Awasthi
Th 25564

*Abstract*
*(Not Verified)*

The afore-mentioned view points and the results of the research work embodied in the thesis entitled "Design, synthesis, characterization and antimalarial activity of newer tetraoxane analogs" are presented in four chapters:Chapter 1 covers the introduction part. In this chapter we have discussed about covalent biotherapy approach. We have discussed the same by taking suitable examples. Additionally, the synthesis and the activity of the various hybrid compounds have been reported. Chapter 2 describes the one-pot synthesis of newer N-sulfonylpiperidine 1,2,4,5-tetraoxane analogs. Then the synthesised 1,2,4,5-tetraoxane analogs were tested for their antimalarial activities against P.falciparum. The results of the characterization and activities against P. falciparum are included.Chapter 3 describes the hybridization approach for the one-pot synthesis of tetraoxane-chalcone hybrid analogs using reductive amination methodology. Later on, the synthesised compounds were tested for their antiplasmodial activities against P. falciparum. The results of synthesis and activities are included.Chapter 4a focuses on the design and synthesis of another series of hybrid analogs containing 1,2,4,5-tetraoxane-thiazole hybrid drugs. The in vitro antiplasmodial activity of these synthesised hybrid analogs is under process. Chapter 4b describes the catalytic activities of amine functionalized SiO2@Fe3O4 nanoparticles for the synthesis of 2-amino-4H-benzo[b]pyrans. The results regarding the better performance of the amine functionalised silica magnetic nanoparticles for pyran synthesis have been included.

*Contents*

1. Chimetic biotherapy as a new strategy in drug design with improved in *vitro* and in *vivo* antiplasmodial activities: an overview 2. Synthesis, structural analysis and in vitro antiplasmodial activity of chemically stable N-sulfonylpiperidine dispiro-1,2,4,5-tetraoxane compounds 3. Reductive amination of substituted chalcones and 1,2,4,5-tetraoxanes using sodium triacetoxyborohydride and their in *vitro* antimalarial activities 4a. Synthesis of hybrid analogs of substituted thiazoles and 1,2,4,5-tetraoxanevia sodium triacetosyborohydride as a reducing agent 4b. Green, mechanochemical, solvent and waste free one-pot multicomponent reaction of 2-amino-4*H*-benzo[*b*]pyrans *via* amine functionalized $Sio_2@Fe_3O_4$ nanoparticles. Summary and Publications.

51. SINGH (Snigdha)

**Synthesis and Development of Novel Heterocycles and their Biological Evaluation.**

Supervisors : Prof. Ramesh Chandra and Prof. Maurizio Taddei

Th 25073

*Contents*

1. Introduction 2. Aim and objectives 3. Benzimidazole-triazole based phthalimides against malaria: *In vivo*, *In vivo* studies and structural activity relationship 4. Synthesis of hydroxyethylamine based piperazine derivatives and biological activities: *In vitro, In vivo*, and structure-activity relationship 5. Fast-acting small molecules targeting malarial aspartyl proteases, plasmepsins, inhibit malaria infection at multiple life stages 6. Syntheis of 8-hydroxyquinoline derivatives as potenrial Gli inhinitors and studies for their conjugation with linker.Summary.Research publications and Conferences/Seminars.

52. SINGH (Vishal)

**Stochastic Dynamics of Protein Misfolding and Aggregation.**

Supervisor : Prof. Prabati Biswas

Th 25075

*Abstract*

*(Not Verified)*

The misfolding and aggregation process is characterized by the conformational transitions of proteins. These transitions are directly related with their functional activity and the initiation of numerous neurodegenerative diseases. Therefore, it is crucial to understand the dynamical aspects of these transitions. In this context, evaluation of the rate constants and Mean First Passage Times (MFPT) of protein misfolding/aggregation is particularly important, as it provides a quantitative estimate of the inherent dynamics and kinetics of misfolding/aggregation. The work presented in the thesis aims to investigate the stochastic dynamics and kinetics of protein misfolding and aggregation. The time evolution of the population of misfolded and aggregated proteins may be modeled in the generalized framework of Master equation, which is based on the principles of stochastic kinetics through rate laws. The Master equation approach is used to calculate the MFPT of protein misfolding and aggregation through simple models. The conformational transitions of proteins may be described as a barrier crossing phenomenon where the passage across the barrier is mediated by random motion of the solvent around the protein. A model of the barrier crossing dynamics of the misfold-fold transition of proteins is described by generalized Langevin equation with a non-Markovian frictional memory kernel in an inverse parabolic potential. The Langevin and Generalized Langevin Dynamics simulation study presented in this thesis investigate the dynamics of conformational transitions of amyloid-beta. These studies reveal the effect of frictional coefficient and height/curvature of the potential barrier on the rate constants, transition path time distribution and mean transition path time of the conformational transitions of proteins. The analytical models and the simulation study presented in this thesis provide an idea about the time required for protein misfolding/aggregation and the factors that influence the conformational transitions of proteins through a multistep equilibria.

*Contents*

1. Introduction 2. Estimating the mean passage time of protein misfolding 3. Predicting protein shelf lives from mean first passage times 4. How barrier highest modulates the misfold-fold transitions of proteins? A generalized langevin equation approach 5. Conformational transitions of amuloid-β: a langevin and generalized langevin dynamics dynamics simulation study. Bibliography.

53. SONAM

**Investigation of Varied Facets of MurB Enzyme and its Inhibitors : An In Silico Approach.**

Supervisor : Prof. Rita Kakkar

Th 25055

*Abstract*

*(Verified)*

This thesis is based on in silico studies of MurB enzyme and its inhibitors. The aim of this thesis is to investigate the active site and conformational aspects of MurB enzyme. Moreover, 4-thiazolidinone derivatives, which inhibit the MurB enzyme, have also been explored for various structural and electronic features. Overall, the thesis is divided into seven chapters. A brief outline is provided below. Chapter 1 (Thiazolidinones: synthesis, reactivity and their biological applications) is a comprehensive review covering aspects like synthesis, reactivity and biological implications of different thiazolidinone derivatives: 2-thiazolidinone, 4-thiazolidinone, 5-thiazolidinone, 2-thioxo-4-thiazolidinone and thiazolidine-2,4-dione. Chapter 2 (Computational Techniques) describes various computer-aided drug design (CADD) techniques and DFT methods. Chapter 3 (A comparative study of the different docking methodologies to accurately assess the protein-ligand interaction for E. coli MurB enzyme) comprises an in silico analysis of the active site of the E. coli MurB enzyme. Two techniques were compared i.e. Glide-XP docking and Induced-fit docking (IFD) and IFD has emerged as the more appropriate for studying the E. coli MurB enzyme. Chapter 4 (Structure-based virtual screening, free energy of binding and molecular dynamics simulations to propose novel inhibitors of the Mtb-MurB oxidoreductase enzyme), focusses on identifying new inhibitors of Mycobacterium Tuberculosis MurB enzyme through structure based virtual screening. Chapter 5 (A theoretical study of the structural features and antioxidant potential of 4-thiazolidinones). In this study, we have explored the antioxidant potential of this five membered 4-thiazolidinone ring using the DFT-B3LYP/6-311(++)G(d,p) method. Chapter 5 (A theoretical study of the structural features and antioxidant potential of 4-thiazolidinones). In this study, we have explored the antioxidant potential of this five membered 4-thiazolidinone ring using the DFT-B3LYP/6-311(++)G(d,p) method. Chapter 7 (Concluding Remarks) summarizes the overall study and a brief description of the scope for future work is also presented.

*Contents*

1. Thiazolidanones: synthesis, reactivity and their biological applications 2. Computational techniques 3. A comparative study of the different docking methodologies to accurately assess the protein-ligand interaction for *E. coli* MurB enzyme 4. Structure-based virtual screening, free energy of binding and molecular dynamics simulations to propose novel inhibitors of the Mtb-MurB oxidoreductase enzyme 5. A theoretical study of the structural features and antioxidant potential of 4-thiazolidinones 6.A theoretical study of the tautomeric transformation and reactivity of 2-amino-4-thiazolidinone 7. Concluding remarks. Bibliography.

54. SUBODH

**Synthesis of Graphene-Metal Oxide Hybrids and Triazine-Based Covalent Organic Polymer Materials for Catalytic and Gas Sensing Applications.**

Supervisor : Dr. Dhanraj T. Masram

Th 25041

*Abstract*

*(Not Verified)*

The present thesis aims to contextualize design and synthesis of two important functional materials; (1) graphene-metal oxide hybrid nano-composites and (2) triazine based covalent organic polymer materials. In brief, a systematic investigation has been performed on these materials to explore their easy synthetic methods and their potential applications in the field of heterogeneous catalysis and sensing. Chapter 1 deals with the introduction to graphene-metal oxide hybrids and triazine-based covalent organic polymer materials. The critical literature review of these two functional materials includes their characteristic properties, and their applications in catalysis and sensing. Chapter 2 includes the synthesis of a new heterogeneous catalyst by chemical modification of graphene oxide (GO) using APTES to achieve the furfural-imine functionality at which copper oxide nanoparticles (NPs) were immobilized. The as-synthesized catalyst was found to be an efficient, and reusable heterogeneous catalyst for the preparation of xanthene derivatives. In chapter 3 we have reported the synthesis of TiO2 NPs based hybrid nanocatalyst via AAPTMS functionalization of GO. The catalyst was evaluated for its catalytic performance towards synthesis of 2,4,5-triaryl imidazoles. Chapter 4 includes the synthesis of a new covalent organic polymer CC-TAPT-COP via poly-(N-arylation) reaction between TAPT and cyanuric chloride. It shows a rapid and naked eye observable response toward HCl vapours, which could be recycled by using ammonia vapours. Further, we found that CC-TAPT-COP acts as a heterogeneous catalyst for synthesis of substituted quinazoline derivatives. In chapter 5, a new micro-spherical covalent organic polymer was synthesized by assembling the two C3 symmetric triazine cored precursors. This COP shows promising solid-state properties along with reversible chromogenic response toward the detection of HCl gas. In chapter 6, silver NPs were immobilized over as synthesized micro-spherical polymer TATF-COM to enhance its catalytic potential for degradation of nitroaromatics describing the significance of shape specific property of COMs.

*Contents*

1. Introduction 2. CuO nanoparticles immobilized over imine functionalized graphene oxide hybrid nanocatalyst for the synthesis of xanthene derivatives 3. $TiO_2$ nanoparticles immobilized organo-reduced graphene oxide hybrid nanoreactor for catalytic applications 4. A new triazine-cored covalent organic polymer for rapid visual detection of HCI gas and catalytic synthesis of substituted quinazolines 5.Chromogenic covalent organic polymer-based microspheres as solid-state gas sensor Silver nanoparticles immobilized covalent organic microspheres for hydrogenation of nitroaromatics with intriguing catalytic activity 7. Conclusions. List of publication.

55. SUMIT KUMAR

**Envisaging the Green Synthesis of Nanoparticles and their Significance on Protein Stability.**

Supervisor : Prof. P. Venkatesu

Th 25060

*Abstract*
*(Not Verified)*

In the current scenario of cut-through technology, the escalation in the field of nanoscience is marvelous for biomedical applications. The classical known methods of NPs synthesis contain surfactants and other toxic materials which enhance the toxicity of NPs disorienting corona formation. Therefore, the green synthesis of gold nanoparticles (AuNPs) has been focused recently to tailor the properties of stability, biocompatibility, and specificity. The fabrication of ILs on AuNPs surface and further qualifying their biocompatibility for protein/enzymes stabilizations has been evaded greatly. Therefore, through this study an attempt has been made to boost the protein stabilization/enzyme immobilization ability of the ILs-AuNPs with ILs and AuNPs synergy. The thesis comprises the protein stability/enzyme immobilization in the presence of two classes of AuNPs; firstly AAIL based AuNPs which show their biocompatibility on the RBCs, Haemoglobin and papain, secondary IL-modified AuNPs which show higher activity and interactions with the Lyz and Cyt-c. Out of AAIL based AuNPs from chapters 3 and 4, the [CHO][Trp]AuNPs prove to be more biocompatible as compare to the [TEA][Trp]AuNPs. Furthermore, from the result of chapters 5 and 6, AuNP-IL2 with methyl sulphate anion has increased the activity of the Lyz and Cyt-c to maximum, respectively. Additionally, the results of chapters 5 and 6 also impart the information of sulphur containing functionalities on the IL-modified AuNPs for the higher compatibility and activity enhancement. Overall results of chapter 3 to 6 conclude that all of AuNPs either AAIL based AuNPs or IL modified AuNPs are biocompatible only at lower concentration and their biocompatibility towards proteins and enzymes tends to decrease with increase in the concentration. Therefore, thorough analysis of all key points related to protein stability in AAIL and IL modified AuNPs have created a new way to modify the various interactions on AuNPs for protein/enzyme immobilization in biomedical applications.

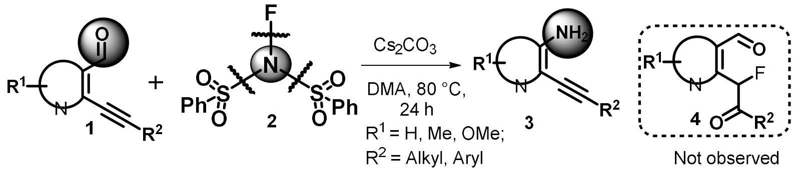
*Contents*

56. SUSHMITA
**A New Aspect of Unsaturated Hydrocarbons for the Construction of *N*-Heterocycles.**
Supervisor: Prof. Akhilesh K. Verma
Th 25043

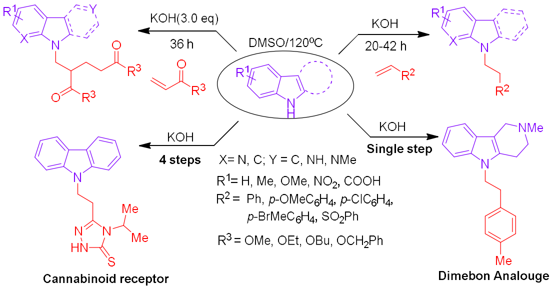
*Abstract*
*(Not Verified)*

**Triple bond Directed Csp$^2$-N Bond Formation Through *N*-Fluorobenzenesulfonimide as Aminating Source: One-Step Transformation of Aldehyde into Amine:** The C-N bond forming reaction attracts the interest of synthetic chemist from the last century as the introduction of amino groups tune the physicochemical properties of the molecule and made them a biologically important structure Traditionally, metal-catalyzed C-N cross-coupling reactions such as Buchwald-Hartwig and Ullmann-type coupling have been exploited for the C-N bond

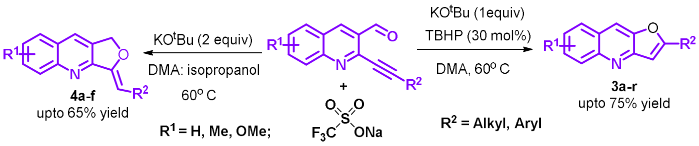
formations. Inspired from our ongoing research on *ortho*-alkynyl aldehydes, herein we hypothesized the synthesis of fluorinated heterocycles through NFSI via metal-free strategy. Our preliminary studies revealed that the reaction failed to afford the proposed fluorinated product, however an aminated productwas isolated.



**2. Olefin-Oriented Selective Synthesis of Linear and Branched *N*-Alkylated Heterocycles *via* Hydroamination:** The C-N bond-forming reactions contribute as one of the most important, versatile and practical synthetic approach for the development of nitrogen-containing compounds that demonstrate numerous applications in natural products and biologically active drugs.[3]Interestingly, heterocycles pendant with *N*-alkyl group enhances the biological activity of the molecule.[4]



**3:Alkyne-Assisted Synthesis of Furoquinolines via Anomalous Dakin-type Reaction**:Furo [3,2-b] Pyridine derivatives are known as TBKl and IKK Inhibitors for the treatment of cancer and also as a melatoninergic activity.Skimmianine, natural alkaloid isolated from rutaceous plant have shown as strong acetylcholinesterase (AChE) inhibitor.6 Due to their extensive medicinal applications, several metal-catalyzed synthetic methodologies are available in literature for their development.



**4: Pd-Catalyzed Buchwald–Hartwig Amination/Cyclization of Quinoxalines: ANew Synthesis of 1,2-diphenyl-1*H*-pyrrolo[2,3-*b*]quinoxaline:** Substituted N, O-heterocycles and their core found in a various natural drugs-like important scaffolds which exhibit wide spectrum of biological activities.[7] Among these various heterocycles quinoxalin and pyrazine cores are significantly applied in pharmaceutically active natural and non-natural compounds.[8] On the basis of this result, we conceived that 1,2-diphenyl-1H-pyrrolo[2,3-*b*]quinoxaline would be manufactured through a Pd- catalyzed one-pot sequential/tandem reaction of 2-chloro-3-(phenylethynyl)quinoxaline with substituted amines.

## *Contents*

1. Triple bond directed *Csp*$^2$-*N*bond formation through *N*-Fluorobenzenesulfonimide as aminating source: one-step transformation of aldehyde into amine 2. Olefin-

oriented selective synthesis of linear and branched *N*-alkylated heterocycles via hydroamination 3.Alkyne-assisted synthesis of furoquinolines via anomalous dakin-type reaction 4. Pd-catalyzed Buchwald-hartwig amination/ cyclization of quinosalines: a new synthesis of 1,2-diphenyl-1H-pyrrolo[2,3-b]quinoxaline. Summary and Copies of publications.

57. SWATI RANI

**Interactive Behaviour of Curcumin in Restricted Molecular Assemblies : A Spectroscopic Study.**

Supervisor : Prof. Subho Mozumdar

Th 25065

*Abstract*

*(Not Verified)*

"Curcumin" is one of the most potentially active hydrophobic substance which is derived from the rhizome of Curcuma longa. Curcumin shows exceptional biomedical applications such as anticancer, anti-inflammatory, anti-oxidant, anti-microbial and anti-diabetic properties. However, in spite of having versatile medicinal applications, curcumin suffers from negative properties such as low aqueous solubility, rapid degradation in neutral as well as alkaline medium and sensitivity towards light. Therefore, attempts have been made to improve the bioavailability of curcumin. There are large number of reports that have been published for the delivery of curcumin using different nano-particulate systems such as liposome, ionic liquids, surfactant, hydrogels, polymeric micelles. But the stability and efficiency of release of curcumin are still some of the major issues that need to be addressed before taking them up for clinical trials. Since, the excited state intramolecular hydrogen transfer (ESIHT) is the major and foremost reason for the instability of curcumin in aqueous media, a complete understanding of the photophysical properties of this drug molecule is undoubtedly necessary to reveal its mechanism of action and binding with different macromolecules and assemblies. It may be mentioned that the photophysics of curcumin in different microenvironment is rapidly becoming an interesting area of research in this country and abroad. The work presented in this thesis mainly focuses on the different nano-delivery systems such as polymeric micelles, surface active ionic liquids and mixed micelles. These have been used for enhancing the solubility and stability of curcumin in an aqueous medium. Further, the photophysics of curcumin inside these microenvironments have been studied by using different optical spectroscopy and other theoretical tools. The complete interaction mechanism of curcumin with these nanoparticulate systems has been investigated and discussed in detail in this thesis.

*Contents*

1. Introduction and review of literature 2. Characterization techniques 3. Solubility and stability enhancement of curcumin in Sorupus® polymetic micelles: a spectroscopic study 4. Effect of pH on the stability and photophysics of curcumin encapsulated Sorupus® micelles 5. Role of imidazolium based SAILs to restrain the ESIHT dynamics of medicinal pigment curcumin: theoretical and experimental approach 6. A detailed insight into the effect of increment in the chain length of RTILs on the photophysics of curcumin-polymeric mecelles 7. Conclusions. Appendices. List of publications.

58. THAKUR (Vasudha)
**Synthetic, Structural and Photophysical/Catalytic Aspects of Cycloplatinated- and Cyclopalladated Guanidines.**
Supervisor : Prof. Natesan Thirupathi
Th 25072

*Abstract*
*(Not Verified)*

2.1.1 The reactions of cycloplatinated 2-anisyl/2-tolyl guanidine complexes, [Pt{κ2(C,N)}X(S(O)Me2)] (X = Cl (1.1.69) and OC(O)CF3 (1.1.71)) with two equiv of 3,5-dimethylpyrazole and 3,5-diphenylpyrazole in toluene afforded the corresponding platinacycles, [Pt{κ2(C,N)}(PzH)2]X (2.1.1-2.1.3) in ≥ 69% yields. The reactions of 1.1.69 with one equiv of 3,5-dmpzH and 3,5-dppzH in the presence of Et3N in toluene afforded the platinacycles, [Pt{κ2(C,N)}(μ-Pz)]2 (2.1.4 and 2.1.5) in 70% and 73% yields, respectively. The reactions of 1.1.69 with one equiv of 3,5-lutidine and 2,6-dimethylphenylisocyanide (L) in CH2Cl2 afforded cis-[Pt{κ2(C,N)}Cl(L)] (2.1.6 and 2.1.7) in 84% and 75% yields, respectively. The reactions of 1.1.69 and 1.1.71 with two equiv of 2,6-dimethylphenylisocyanide in the presence of one equiv of AgBF4 afforded cationic platinacycles, [Pt{κ2(C,N)}L2]BF4 (L = C=NAr, Ar = 2,6-Me2C6H3; 2.1.8 and 2.1.9) in 81% and 77% yields, respectively. 2.3.1 We report a straight forward high yield syntheses and complete characterisation of two dinuclear cycloplatinated guanidinate(2-) complexes 2.3.2 and 2.3.3 wherein the ligand revealed an unprecedented tridentate μ2-κ2(C,N):κ1N coordination mode as revealed by single crystal X-ray diffraction. A plausible mechanism for the formation of 2.3.2 and 2.3.3 is outlined.2.4.1 The reactions of N,N',N'-tri(4-tolyl)guanidine with Pd(OC(O)Me)2 and N,N',N'-tris(2-anisyl)guanidine with Pd(OC(O)tBu)2 in toluene afforded six-membered cyclopalladated guanidines, [Pd{κ2(C,N)}(μ-OC(O)R)]2 (2.4.1 and 2.4.2) in 71% and 78% yields. The reactions of 2-anisyl and 2-tolyl derived known palladacycles [Pd{κ2(C,N)}(μ-X)]2 (X = OC(O)CF3 (1.2.23) and Br (1.2.33)) with 2 equiv of PPh3 carried out separately in CH2Cl2 at RT for 24 h afforded cis-[Pd{κ2(C,N)}X(PPh3)] (2.4.3 and 2.4.4) in 87% and 83% yields respectively. Palladacycle 1.2.22 was used as catalyst in SMCR involving PhB(OH)2 and aryl bromides/aryl chlorides with 0.01 mol% catalyst loading and the coupling products were obtained in >90% yields in each case.

*Contents*

1. Introduction 2. Results and discussion 3. Supporting information.

59. TIWARI (Ankit)
**Oxidative Functionalization and Annulation Strategies for Construction of Bicyclic and Polycyclic Nitrogen-Containing Heterocycles.**
Supervisor : Dr. K. Gapalaiah
Th 25036

*Abstract*
*(Not Verified)*

The work complied in this thesis basically based on the contemporary concepts of synthetic organic chemistry by keeping the traditional principles of preparative chemistry which are as follow: (i) First chapter describes the iron(II)-catalyzed stereoselective oxidative condensation of indolin-2-ones with benzylamines to synthesize the (E)-3-benzylideneindolin-2-ones; (ii) Second chapter deals with

iron(II)-catalyzed C-H hydroxylation of 1,2-diphenylethane into benzil followed by condensation with 1,2-diaminobenzenes for the preparation of 2,3-diphenylquinoxalines; (iii) Third chapter discloses the copper(I)-catalyzed oxidative annulation of 2-aminobenzylalcohols with 1,2,3,4-tetrahydroisoquinoline for preparation of 5H-isoquinolino[1,2-b]quinazolin-8(6H)-ones; (iv) Fourth chapter describes the modular synthesis of 6-aryl-5H-quinazolino[4,3-b]quinazolin-8(6H)-ones through copper(I)-catalyzed one-pot sequential cross-dehydrogenative annulation of 2-aminobenzamides, 2-aminobenzylalcohols and benzylamines; (v) Fifth chapter deals the preparation of 6-aryl-5H-quinazolino[4,3-b]quinazolin-8(6H)-one by copper(I)-catalyzed one-pot sequential oxidative condensation of 2-aminobenzamides, 2-aminobenzylamines and benzylamines. In first chapter, we have explored an efficient and stereoselective iron(II)-catalyzed reaction for the construction of (E)-3-benzylideneindolin-2-ones from readily available indolin-2-ones and benzylamines and FeBr2 as catalyst. In second chapter, we have developed a novel one-pot sequential cascade method for the preparation of 2,3-diphenylquinoxalines via iron-catalyzed C-H hydroxylation of 1,2-diphenylethane followed condensation with 1,2-diaminobenzene. In chapter three, we devised an efficient oxidative annulation for the formation of ring-fused quinazolinone scaffolds which are the core structures of numerous bioactive molecules as well as alkaloids from easily available starting materials. Copper(I)-bromide drives this oxidative annulation between 1,2,3,4-tetrahydroisoquinoline and 2-aminobenzylalchols to produce the 5H-isoquinolino[1,2-b]quinazolin-8(6H)-ones in moderate to excellent yields. In chapter four, we have studied a cascade annulation method for the synthesis of 6-aryl-5H-quinazolino[4,3-b]quinazolin-8(6H)-ones via copper(I)-catalyzed one-pot sequential annulation by employing 2-aminobenzamides, 2-aminobenzylalchols and benzylamines. In chapter five, we have presented a convergent method for accessing 6-aryl-5H-quinazolino[4,3-b]quinazolin-8(6H)-ones through copper(I)-catalyzed oxidative annulation of 2-aminobenzamides, 2-aminobenzylamines and benzylamines using one-pot sequential strategy.

*Contents*

60. URVASHI

**Transition-Metal-Catalyzed C-C/C-S Coupling and C-N Bond Formation: Synthesis of *N*-Heterocyclic Compounds and their Biological Evaluation.**

Supervisor : Prof. Shrikant Kukreti and Prof. Vibha Tandon

Th 25057

*Abstract*
*(Not Verified)*

The main focuses : a) a wide functional group or substituents tolerance; b) regio, stereo, and chemoselectivity for functionalization; c) late stage functionalization; d)

optimization synthesis, milder conditions; e) to facilitate one pot strategies; f) to avoid use of expensive reagents, solve challenging product separations. Chapter 1: Synthesis of 1,2-dihydroisoquinolines via a 6-endo dig cyclization using direct nitro Mannich condensation using inexpensive cobalt chloride, resulting high yields. Plausible mechanism based on via isoquinolinium intermediate is proposed. Chapter 2 : Synthesis of 1,2- dihydroisoquinolines having different functionality at the C-1, C-3, C-7, and N-2 positions for evaluation against HIV-1 integrase (HIV1-IN) inhibitory activity. Two molecules as potent integrase inhibitors in in vitro strand transfer (ST) assay, with IC50 = 0.7 and 0.8 μM, respectively obtained. Molecular docking confirmed molecules stabilizes the enzyme−inhibitor complex. Antiviral assay shows the reduction of the level of p24 viral antigen by 91%. Interestingly, Similar ST inhibitory activity in G140S mutant also achieved. Chapter 3: Synthesis of diarylpyrazolo[3,4-b]pyridine from combination of chemoselective Suzuki–Miyaura cross-coupling reactions and then in a one-pot manner without much loss of efficiency showing applicability to aryl/heteroaryl-boronic acids with high selectivity of the C3 over the C6 position. Chapter 4 : DABSO mediated sulfonylation of 7-azaindoles via sulfonylative Suzuki-Miyaura cross coupling (SMC) reaction giving C-3 sulfonylated azaindolyl derivatives. Involvement of in-situ generation of ArSO2 free radical followed by the key steps of SMC reaction has been discovered and proposed mechanism supported by Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) calculations.

*Contents*

1. An expedient approach to 1,2-dihydroisoquinolines derivatives *via* cobalt catalysed mannich condensation/6- *endo dig* cyclisation of *o*-alkynylarylaldimines 2. Design, synthesis and biological evaluation 1,2-dihydroisoquinolines as HIV-1 integrase inhibitors 3. Palladuim (II) catalysed sequential and one-pot sequential Suzuki-miyaura coupling for the synthesis of 3,6 diaryl-1*H*-pyrazolo[3,4-*b*]pyridines 4. Cu(II)-catalyzed sulfonylation of iodo substituted-7-azaindoles using DABSO as $SO_2$-source and its mechanistic study. Publications.

61. VERMA (Shalini)

**Exploiting the Reactivity of Alkynes towards the Construction of Novel Heterocyclic Entities.**

Supervisor : Prof. Akhilesh K. Verma

Th 25045

*Abstract*

*(Not Verified)*

We have developed an efficient approach for the synthesis of functionalized tetrahydro-pyrido/quinolinocarbazoles from 2-alkynylindole3-carbaldehydes and L-proline utilizing a metal-free decarboxylative cyclization, ring expansion, and ring contraction strategy via the generation of azomethine ylide was developed. The reaction of 2-alkynylindole-3-carbaldehydes with L-thioproline leads to the formation of γ-carbolines. By virtue of this expedient method, a diverse range of biologically active heteroannulated carbazoles can be synthesized efficiently. Further, metal-free regioselective hydration of o-alkynylaldehydes with the assistance of neighboring carbonyl oxygen is disclosed. The developed protocol provides a facile route to synthesize a series of multisubstituted carbonyl containing scaffolds that enable the potential application toward the synthesis of highly diversified 5-azaindoles. γ-Carbolines and 2,8- diazacarbazoles can also be accessed directly without isolating the dicarbonyl compounds. The developed methodology is operationally simple and environment-friendly, tolerates a wide variety of functional groups, and is applicable toward large scale synthesis. Next we carry out a transition-metal-free approach for construction of nitronaphthylamines for the first time through aza-henry, chemoselective, and regioselective annulation of 2-alkynylbenzonitriles with nitromethane. In addition, the strategy provides an elegant, operationally simple and atom-economical route for the synthesis of nitroamino substituted heterocyclic scaffolds, featuring a range of sensitive functional groups. The reaction could also devise acetonitrile and acetophenone as nucleophile. The protocol has been successfully implemented for late-stage modification of bioactive molecules. Furthermore, a base-mediated versatile cascade annulation/formylation of 2-alkenyl/alkynylbenzonitriles with 2-methylbenzonitriles has been established for the construction of four different classes of amino and amido substituted benzo[c]phenanthridines and benzo[c]phenanthrolines. The transformation utilizes the solvent DMF as the formyl source for the synthesis of amido-substituted scaffolds. This strategy allows the formation of multiple C-C and C-N bond formation in one pot at room temperature.

*Contents*

1. Transition-metal-free access to pyridocarbazoles from alkynylindole-3-carbaldehydes *via* azomethine ylide 2. Metal-free carbonyl-assisted regioselective hydration of alkynes: an access to dicarbonyls 3. Aza0henry reaction: synthesis of nitronaphythylamines from 2-(Alkynyl)benzonitriles 4. Base-mediatyed annulation of alkenyl/alkynylbenzonitriles: an unified approach to benzo[*c*]phenanthridines. Summary of the work. Copies of the publications.

62. VISHVAKARMA (Vijay Kumar)
**A Computational Approach to Study the Potential of Thiazolidines for the Inhibition of NS2B-NS3 Protease of Dengue Virus.**
Supervisor: Dr. Prashant Singh
Th 25068

*Abstract*
*(Verified)*

Dengue fever (DENF) is caused by the infection of dengue virus (DENV). DENV is mainly spread by the biting of infected mosquito, mainly Ades aegypti and some lesser extent to Ades albopictus. DENF is characterized by fever with a sudden decrease in platelet count. As a result composition of blood is destroyed and the patient may dies. Till date, there is no effective medicine to cure the patient from DENV infection. However, only symptoms of DENF have been treated by the physicians. The majority of the marketed drugs to cure different fever contain heterocyclic rings. Thiazolidines is a five-membered ring and contains nitrogen and sulfur. They have shown different biological properties like antimicrobial, antiviral, antibiotic, etc. In this thesis, eight (AH) potent thiazolidines have been designed via one-pot multicomponent reaction and the feasibility of the synthesis of A-H was studied by the density functional theory (DFT) methods. Further, a library of compounds based on A-H is designed and screened through molecular docking and ADMET (absorption, distribution, metabolism, excretion and toxicity). Further, the top six screened thiazolidines were analyzed by the DFT analysis. Finally, molecular dynamics (MD) simulation and molecular mechanics energies combined with the Poisson–Boltzmann and surface area (MM-PBSA) analysis of the NS2B-NS3 protease of DENV with and without top six thiazolidines were performed. The anchoring of these thiazolidines within the active binding cavity of the NS2B-NS3 protease of DENV is analyzed by the number of H-bonds forms between potential thiazolidines and the amino acid residues of the active binding cavity. The binding energy pattern obtained from MD simulation and MM-PBSA analysis of the top six thiazolidines were correlated to each other to refine the result towards accuracy.

*Contents*

1. Review of literature 2. Objectives of the thesis 3.Scheme, their mechanism and density functional theory 4.Docking, screening and density functional theory analysis 5.Absorption, distribution, metabolism, excretion and toxicity analysis 6.Molecular dynamics simulation and molecular mechanics poisson-boltzmann surface area analysis 7. Summary 8.Reprint of articles.