

## CHAPTER 10

### CHEMISTRY

#### Doctoral Theses

01. ADHESH KUMAR  
**Role of Local, Nonlocal Interactions and Correlated Mutations in Misfolding Proteins.**  
Supervisor: Prof. Prabati Biswas  
Th 24382

*Abstract*  
(Verified)

A Monte Carlo simulation based sequence design method is used to design sequences for Ca chain backbones of real proteins. A statistical potential is developed from the compilation of a data set of proteins. The designed sequences are misfolded by tuning local and nonlocal interactions through both site-directed point and correlated pair mutations. This protein design approach is used to explore the attributes of these misfolded sequences using different statistical techniques. The role of the local and the nonlocal interactions in protein folding, misfolding and unfolding is investigated. The effect of site-directed point and correlated pair mutations on the stability of proteins is explored. Optimization of the local interactions may hold the key to design sequences with less misfolding propensity. The methods presented may be used to identify specific site-directed mutation patterns for estimating and comparing the mutability of different amino acid residues in different structural contexts for the folded and misfolded conformations of proteins.

*Contents*

1. Introduction 2. Role of local and nonlocal interaction in folding and misfolding of globular proteins 3. Effect of site-directed point mutations on protein misfolding simulation study 4. Effect of correlated pair mutations in protein misfolding. Bibliography.

02. ANUJ KUMAR  
**Exploration of Perovskite Oxides Based on Anion-Intercalation for Pseudocapacitive Charge Storage.**  
Supervisor: Dr. Raj Kishore Sharma  
Th 24919

*Abstract*  
(Not Verified)

Perovskite oxides are class of materials those store the charge through anion intercalation mechanism. The present thesis explains the different crystal structure and utilization of perovskite oxides as supercapacitor electrode materials. Supercapacitors deliver energy at a high rate owing to restricted diffusion limitations process but it suffers from low energy density. Therefore, a little-know mechanism i.e anion intercalation mechanism is studied thoroughly using different

perovskite oxides. High oxygen vacancies, ion mobility, and structural stability are the three main parameters that directly affect supercapacitors properties. The presence of inherent oxygen vacancies promotes anion intercalation mechanistic path (fast kinetic) that does not involve a phase transition. Moreover, perovskite structures have the ability to accommodate electrolytic ions while maintaining structural integrity. In the entire thesis, different perovskite crystal structures are explored such as simple perovskite, doped perovskite, double perovskite, and triple perovskite. In the whole work, B-site of the perovskites is modified either by doping or by taking an equal ratio of different redox-active metals for enhancement of charge storage. Depends on their electrochemical study, triple perovskite performance surpassed all of them in terms of capacitance, energy density, and power density supercapacitive metrics. During the double perovskite oxide study, it is also explained how to choose B-site elements to fabricate high-rate supercapacitors. Other than this, it is also discussed how we can synthesize high-voltage aqueous supercapacitor using different B-site cations. Based on the charge storage mechanism, an improved understanding of the role of constituent elements is also discussed for further modification in charge storage characteristics. Besides, fast kinetic based mechanistic charge storage ensures excellent cycling stability by prohibiting phase transformation.

#### *Contents*

1. Introduction 2. Characterization techniques for supercapacitive materials 3. SrTiO<sub>3</sub> perovskite oxide as high performance aqueous as well as flexible solid-state supercapacitor cell 4. Mo-doped strontium cobaltite perovskite oxide as an anion-intercalation supercapacitor electrode with high energy density 5. B-site cation ordered Sr<sub>2</sub>CoMoO<sub>6-δ</sub> double perovskite as high-rate anion intercalation pseudocapacitance 6. Triple perovskite as an advanced pseudocapacitive material: multifarious element approach with ordered structure 7. Conclusion .List of publications.

03. AGARWAL (Drishti)

**Evaluation of the Antimalarial Potential of Novel Synthetic Small Molecules.**

Supervisor: Prof. Stish K. Awasthi

Th 24404

#### *Abstract* (Not Verified)

Chapter I comprises the Review of Literature: “From Artemisinin-based Combination Therapy (ACT) to the newer hybrid approach: stepping up the malaria movement” Effort has been made to cover all major aspects encompassing antimalarial artemisinin combination therapy (ACT), including the benefits and pitfalls of the major available ACTs recommended as first-line therapy, and how they are being fine-tuned to develop new, promising combinations, under various stages of clinical development. Chapter II describes the “In vitro and in vivo antiplasmodial activity of aminoquinoline derivatives against chloroquine-resistant parasites” These new derivatives are potent against CQ resistant *P. falciparum* parasites. The compounds were tested: (i) as blood schizonticides against *P. falciparum* in vitro; (ii) against *P. berghei* infections in mice; (iii) for their in vitro cytotoxicity; (iv) in vivo toxicity; (v) for their binding mode to lactate dehydrogenase and dimeric hemozoin in silico. In Chapter III, “Antiplasmodial synergistic interaction of fluoroquinolone analogues in combination with artemisinin; their curative effect in rodent malaria model” we investigated the fixed-ratio combinatorial interactions of three novel fluoroquinolone

derivatives with artemisinin, for treating the erythrocytic stages of *P. falciparum* 3D7. A modified isobologram method was followed to assess the synergistic, antagonistic or additive interactions. Further, we assessed their efficacy in vivo, employing a rodent malaria model. Chapter IV is entitled “Elucidating the mechanism of action of novel benzimidazole derivatives against *Plasmodium falciparum*”. It highlights the employment of DNA gyrase as a potential chemotherapeutic target. Our benzimidazole derivatives show remarkable in vitro anti-plasmodial activity. Their IC<sub>50</sub> values are in single-digit, micro-molar range. They display potent inhibition of bacterial DNA gyrase catalytic activity and cause inhibition of gyrase-DNA complex formation, due to binding of the compound to DNA fragment. UV-visible spectroscopy confirmed the binding of compound with DNA, which was further validated by molecular docking with the DNA helix.

#### *Contents*

1. Review of literature from artemisinin- based Combination therapy (ACT) to the newer hybrid approach: stepping up the malaria movement 2. In vitro and in vivo antiplasmodial activity of aminoquinoline derivatives against chloroquine-resistant parasites 3. Antiplasmodial synergistic interaction of fluoroquinolone analogues in combination with artemisinin; their curative effect in rodent malaria model 4. Elucidating the mechanism of action of novel Benzimidazole derivatives against *Plasmodium falciparum*. Summary. List of publication.

04. AGARWAL (Shalini)  
**Catalytic Approaches for synthetic Transformations in Organic Chemistry.**  
 Supervisor: Prof. Mahendra Nath  
Th 24393

#### *Abstract (Verified)*

The objective of this dissertation is to develop green catalytic protocols for the facile, convenient and efficient synthesis of various biologically important heterocyclic compounds. The work presented in this thesis is divided into five chapters. The first chapter of this thesis presents a brief account on the importance of green chemistry, catalysis and green solvents for carrying out various organic transformations. Chapter 2 discusses the zinc proline hybrid material catalyzed eco-friendly and versatile strategy for the synthesis of 2,4,5-triaryl- and 1,2,4,5-tetraarylimidazoles via one-pot condensation of benzil or benzoin with various aromatic/heteroaromatic aldehydes and ammonium acetate or/and aromatic amines. Chapter 3 describes a green and rapid approach for the one-pot domino Knoevenagel-Michael synthesis of bis-cyclohexenones and 1,8-dioxooctahydroxanthenes employing caffeine hydrogen sulfate as a green acid catalyst at different temperature conditions. Chapter 4 deals with caffeine hydrogen sulfate assisted efficient and environmentally benign strategy for the preparation of densely functionalized spiroxyindoles via one-pot condensation of isatins, malononitrile and different activated carbonyl compounds. Chapter 5 presents a facile and green protocol for one-pot aqueous synthesis of 2-aminothiazoles in the presence of catalytic amount of sulfonic acid functionalized magnetic zinc ferrite nanoparticles at room temperature. The discussed synthetic protocols unveiled several potent and wonderful catalytic systems for various eco-compatible organic transformations and provided promising opportunities for sustainable development of green and eco-friendly chemistry.

*Contents*

1. Green chemistry and catalysis 2. Environmentally benign synthesis of 2,4,5-triaryland 1,2,3,4,5-tetraarylimidazoles using a hybrid material catalyst 3.Green and efficient approach one-pot domino knoevenagel-michael synthesis of cyclohexenones and 1,8-dioxooctahydroxanthenes 4.Facile and green synthesis of functionalized spiroxyindoles using caffenium hydrogen sulfate as a catalyst 5. Nainoprticles catalyzed green approach for one- pot synthesis of 2-aminothiazoles in water.Summary. Publication & conferences.

05. AMAR ABDEL RASHED ABDEL KADER MOHAMED ELAGAMY  
**New Strategies for the Synthesis and Functionalization of Butenolides & Chromones.**  
 Supervisor: Dr. Ramendra Pratap  
Th 24386

*Abstract*  
*(Not Verified)*

We have developed new strategies for the synthesis of novel butenolides and chromones. Further, their synthetic applications were carried out to afford other modified derivatives. The outcome of the whole work is described in the following chapters. Chapter 1 provides an efficient synthetic route to functionalized butenolides and spirobutenolides via nitroalkane-mediated ring contraction of 2H-pyran-2-ones/2-oxobenzo[h]chromenes through denitration. When nitroethane was used as a nucleophile source in lieu of nitromethane, it provides (E)- and (Z)-isomer of spirobutenolides in different ratio depending on the substitution pattern using 2-oxobenzo[h]chromenes while, only (E)-isomer of butenolides was obtained using 2H-pyran-2-ones. Most interesting finding in this reaction is base-mediated chemoselective allylic denitration. In Chapter 2, conjugated trienes were synthesized via decarboxylative rearrangement of suitably functionalized butenolides and spirobutenolides. The mixture of the (E)- and (Z)-isomer of spirobutenolides undergoes decarboxylative rearrangement in presence of sodium ethoxide as a base to yield (E)-isomer of trienes. While, (E)-isomer of butenolides proceed to give a mixture of (2E,4E)- and (2E,4Z)-isomer of trienes in almost steady ratio of 45:55 or (1:1.2). In Chapter 3, a new synthetic approach to 2-(methylthio)-4H-chromen-4-ones was developed via oxidative cyclization of  $\alpha$ -aroylketene dithioacetals under mild conditions. Mechanistically, we have observed that iodine has promoted the cyclization of  $\alpha$ -aroylketene dithioacetals through radical pathway. Bromination and chlorination of 4H-chromen-4-ones at the C-3 position were achieved through nucleophilic substitution reaction. In addition, DDQ and I<sub>2</sub> were employed to access 3-iodinated chromones. In chapter 4, flavones were achieved by sulfide and selective sulfide Liebeskind-Srogl cross-coupling reaction of 2-(methylthio)-4H-chromen-4-ones and 3-halo-2-(methylthio)-4H-chromen-4-ones with arylboronic acids. This method is the first example of employing Liebeskind-Srogl coupling for the synthesis of flavones. In addition, various kinds of chemical reactions were conducted to demonstrate the utility of 2-(methylthio)-4H-chromen-4-ones.

*Contents*

1. Nitroalkane-mediated ring contraction of 2H-Pyran-2-ones/2-oxobenzo[h]chromenes through denitration:an efficient synthetic route to functionalized butenolides and spirobutenolides 2. Synthesis of highly-substituted conjugated trienes via decarboxylative rearrangement of suitably functionalized butenolides and

spirobutenolides 3. Development of new methodology to access halogenated and thiomethylated 4H-Chromen-4-ones 4. Transition metal-catalyzed and metal-free modification of functionalized 2-(methylthio)-4H-chromen-4-ones. List of publication

06. BAHUGUNA (Aprana)  
**Computational Approach for the Development of Antitubercular and Antimalarial Agents.**  
 Supervisor: Prof. Diwan S. Rawat  
Th 24397

*Abstract*  
 (Not Verified)

Chapter 2: 3D QSAR studies on cationic amphiphilic indole derivatives for antimycobacterial agents. This chapter describes field-based 3D quantitative structure-activity relationship (3D-QSAR) studies of 79 amphiphilic indole derivatives. The derived 3D-QSAR models showed acceptable R<sup>2</sup> (0.91) and Q<sup>2</sup> (0.91) with an RMSE of 0.08. New molecules with the potential of showing better antimycobacterial activity were designed. Chapter 3: Prediction of three-dimensional structure of M. tuberculosis QcrB protein using homology modelling. This chapter includes building a three-dimensional structure of M. tuberculosis QcrB protein using homology modeling by MODELLER (<http://salilab.org/modeller/9v7/manual/node8.html>). In an attempt to exactly understand the interaction of Q203 with QcrB protein we predicted the 3-dimensional structure of QcrB. Chapter 4: Molecular insights into the interaction of PfDHFR and 4-aminoquinoline pyrimidine based molecular hybrids: Docking studies and ADME prediction. To analyze the interactions of novel 4-aminoquinoline-pyrimidine hybrid compounds with Pf-DHFR-TS we tried to dock the hybrid compounds synthesized in our laboratory into the X-ray structures of wild type Pf-DHFR-TS and quadruple mutant Pf-DHFR-TS. Molecular docking studies of the highest active compounds (IC<sub>50</sub> < 1 μM) obtained from in vitro studies, were performed in the binding site of both the wild type Pf-DHFR-TS (PDB ID:3QGT) and quadruple mutant Pf-DHFR-TS (PDB ID:3QG2) crystal structures. The results clearly indicate that the most active compounds in the study exhibited significant binding affinities as is evident from their Glide energies obtained on docking with the wild (Glide energy range -60.28 kcal mol<sup>-1</sup> to -51.67 kcal mol<sup>-1</sup>) as well as quadruple mutant (Glide energy range -59.11 kcal mol<sup>-1</sup> to -52.74 kcal mol<sup>-1</sup>).

*Contents*

1. An overview of new anti-tubercular drugs, candidates and their targets 2. 3D QSAR studies on cationic amphiphilic indole derivatives as antimycobacterial agents 3. Prediction of three-dimensional structure of M. tuberculosis QcrB protein using homology modelling 4. Molecular insights into the interaction of PFDHFR and 4-aminoquinolinepyrimidine based molecular hybrids: docking studies and ADME prediction. List of publication. Conferences and workshops.
07. BARTWAL (Gaurav)  
**Ampyrone based azo dyes for selective sensing of ph and metal ions (Al<sup>3+</sup>, Co<sup>2+</sup>, Th<sup>4+</sup>), synthesis of coumarin based bis-oxazines and applications of nickel boride**  
 Supervisor: Prof. J.M. Khurana  
Th 24398

*Abstract*  
(Not Verified)

This thesis entitled “Ampyrone based azo dyes for selective sensing of pH and metal ions ( $Al^{3+}$ ,  $Co^{2+}$ ,  $Th^{4+}$ ), synthesis of coumarin based bis-oxazines and applications of nickel boride” synthesis of novel fluorescent probes for selective detection of metal ions. Additionally, a catalyst free synthesis of oxazines using MCRs approach and nickel boride mediated chemoselective deprotection of 1,1-diacetates and reduction of aryl diazonium tetrafluoroborates have been reported. The subject matter of the thesis has been divided into five chapters. Chapter I consists of two parts. In part A, we have reported the synthesis of a novel azo dye 4-((6-hydroxybenzo[d][1,3]dioxol-5-yl)diazenyl)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one and its role as a selective aluminium ions and pH sensor. Application of another phenol-ampyrone based azo dye as a colorimetric/fluorescent probe for selective  $Al^{3+}$  ion detection has been reported in Part B. Chapter II describes application of a novel rhodamine functionalized dye, (3',6'-bis(diethylamino)-2-((Z)-(5-((E)-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)diazenyl)-2,4-dihydroxy benzylidene)amino) spiro [1H-isoindoline-1,9'-[9H]xanthen]-3(2H)-one, as a selective pH switchable colorimetric/fluorescent probe for detection of  $Th^{4+}$  ions. Chapter III consists of two parts. Part A describes synthesis of 6-hydroxyquinoline based azo dye, (E)-4-((6-hydroxyquinolin-5-yl)diazenyl)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one, and its role as a selective sensor for aluminium and hydroxyl ions. Part B includes application of 8-hydroxyquinoline based azo dye, (E)-4-((8-hydroxyquinolin-5-yl)diazenyl)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one, as a selective probe for cobalt and hydroxyl ions. Chapter IV has described a facile synthesis of 3,7-diaryl-12-methyl-3,4,7,8-tetrahydro-2H-chromeno [6,5-e:8,7-e']bis([1,3]oxazine)-10(6H)-ones by one-pot three component condensation of 5,7-dihydroxy-4-methyl-2H-chromen-2-one, aromatic amines and formaldehyde in ethanol at room temperature. Chapter V consists of two parts. Part A describes chemoselective deprotection of 1,1-diacetates to aldehydes and deprotection with concomitant reduction to alcohols with nickel boride, generated in situ from nickel chloride and sodium borohydride in methanol. Nickel boride mediated chemoselective reduction of aryl diazonium tetrafluoroborates to corresponding aryl hydrazines and aryl amines has been reported in part B. Chapter VI describes summary and conclusions of the work reported in this thesis.

*Contents*

1. Synthesis characterization and application of ampyrone based PET-active azo dyes as colorimetric and fluorescent probes for  $Al^{3+}$  ions 2. Synthesis characterization and application of rhodamine functionalized azo-phenol dye as a selective pH switchable colorimetric/fluorescent probe for detection of  $Th^{4+}$  ions: implication towards multiple logic gates 3. Quinoline – ampyrone functionalized azo dyes as colorimetric and fluorescent enhancement probes for selective detection of  $Al^{3+}$  and  $Co^{2+}$  ions in semi-aqueous media 4. A catalyst free synthesis of coumarin functionalized bis-oxazines in ethanol at room temperature 5. Nickel boride mediated deprotection of 1,1-diacetates and reduction of aryl diazonium tetrafluoroborates. Summary and conclusions. List of publication.

08. BHAKUNI (Kavya)  
**Macromolecular Crowding Effect on the Structural Stability and Activity of Proteins : A Biophysical Study in Various Ionic Liquid Media**  
 Supervisor: Dr. P. Venkatesu  
Th 24407

*Contents*

1. Introduction and literature review 2. Materials and methods 3. Crowded milieu tuning the stability and activity of stem bromelain 4. Designing biological fluid inspired molecularly crowded ionic liquid media as sustainable packaging platform for cytochrome c 5. Exploring the counteracting and refolding ability of choline based ionic liquids towards dextran perturbed HAS structure 6. Envisaging the structural and thermal stability of bovine serum albumin in presence of crowders, deep eutectic solvent and their combination. Conclusion.

09. BHASKARAN

**Corrosion Mitigation of Mild Steel in Acidic Medium by Imidazolium Ionic Liquids**

Supervisor: Prof. Gurmeet Singh

Th 24396

*Abstract*  
(Not Verified)

Anticorrosion impact of green ionic liquids (ILs) [MNBIm]Br, [BMBIm]Br, [EOMIm]Br, [DMIm]Br, [FBMIm]Br, [DFBMIm]Br, [MPFMIm]Br have been studied for mild steel in 0.5 M H<sub>2</sub>SO<sub>4</sub> solution using computational and electrochemical methods. The structures of the obtained ILs were confirmed by using <sup>1</sup>H NMR, <sup>13</sup>C NMR, and FTIR spectroscopy, which also confirm the absence of any major impurity. The adsorption of the ILs on the mild steel surface nicely follows Langmuir adsorption isotherm. The corrosion data extracted from Tafel plots and electrochemical impedance spectroscopy (EIS) indicate quite high inhibition effectiveness at acidic pH levels. Polarization curves also suggest that the IL molecules show a mixed mode of mitigation. Scanning electron microscopy (SEM), Energy Dispersive X-Ray Analysis (EDX) and atomic force microscopy (AFM) observations of mild steel surface confirmed the existence of protective inhibitor film on metal surface in the presence of the ILs. The computational descriptors given by density functional theory (DFT) of the IL molecules have also supported the experimental findings within the satisfactory limits and strengthened the overall studies. The interactions of ILs with the metal substrate are obtained using Schrodinger – Materials Science Suite version 2018-3 (MS-Suite) using advanced molecular dynamics simulation. The computational descriptors given by density functional theory (DFT) and advanced molecular dynamics (MD) simulation of the present molecules have also supported the experimental findings within the satisfactory limits and strengthened the overall study.

*Contents*

1. Introduction 2. Review of literature 3. Experimental procedure 4. Synthesis of ionic liquids 5. Galvanostatic polarization studies 6. Electrochemical impedance spectroscopy (EIS) 7. Temperature kinetics studies 8. Surface morphological studies 9. Quantum chemical calculations 10. Conclusion. List of publication. Conferences attended .

10. TOMAR (Ravi)

**Development of Cerium Based Heterogeneous Catalysts: Application in Organic Synthesis.**

Supervisor: Prof. Ramesh Chandra

Th 24408

*Abstract*  
(Not Verified)

Cerium based materials are versatile and robust catalytic material with surface acid-base properties and structure that can be nicely tuned by doping with transition or rare earth metals. There has been an increasing attention to synthesize cerium based heterogeneous catalysts and employing them in organic synthesis as new catalytic systems. In this doctoral thesis, we have designed four different cerium based catalysts such as hybrid Mg(OH)<sub>2</sub> and CeCO<sub>3</sub>OH composite, (2) Pd(OAc)<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>/MgCe-HDC, (3) hybrid Mg(OH)<sub>2</sub>&CeO<sub>2</sub> composite and (4) CeO<sub>2</sub>/HT that were found to be effective in the organic transformation reactions like Henry reaction, oxidation of alcohols, direct imine formation, Knoevenagel condensation, Suzuki-Miyaura Coupling reaction. We have characterized them by using different techniques including FT-IR, TGA/DTA, XRD, UV-Vis, XRD and BET. The present work was divided into five chapters. Firstly, we have used hybrid Mg(OH)<sub>2</sub> and CeCO<sub>3</sub>OH composite for solvent-free Henry reaction at room temperature. Thereafter, hybrid Mg(OH)<sub>2</sub> and CeCO<sub>3</sub>OH composite used as support for Pd(II) salt and then, derived Pd(OAc)<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>/MgCe-HDC catalyst was used for base-free Suzuki- Miyaura coupling reaction in water. Next, hybrid Mg(OH)<sub>2</sub> and CeO<sub>2</sub> composite was used for three organic transformation (oxidation of alcohols, imines formation, and Knoevenagel condensation). In the later step, CeO<sub>2</sub>/HT catalyst was used in oxidation of alcohols and direct imine formation from alcohols in air. Synthesized catalysts and their potential applications are depicted in the diagram. In conclusion, this study paves way to design and develop new catalytic routes for organic transformation using various cerium based catalysts and characterized by different techniques. We have successfully employed these catalysts for the potential applications in chemical industries and scientific community. In view of future prospective, presented catalysts possess important use in biomass conversion into value added compounds, oxidation of HMF, and so on.

*Contents*

1. Introduction 2. Synthesis and characterization of magnesium hydroxide and cerium carbonate hydroxide composite and application in Henry reaction 3. Palladium (II) supported catalyzed base-free Suzuki-Miyaura coupling in water 4. Synthesis and characterization of magnesium hydroxide and cerium oxide composite with application in organic reactions 5. Hydrotalcite supported ceria nanoparticles as heterogeneous catalyst for one-pot synthesis of imines under atmospheric air. Summary.

11. CHAURASIA (Madhuri)  
**Synthesis, Spectral Characterization, Theoretical Studies and Applications of Transition Metal Complexes of Schiff Base Ligands.**  
 Supervisor: Dr. Sulekh Chandra  
Th 24399

*Abstract*  
(Not Verified)

The metal-based drug has gained much attention due to their wide applications in the field of medicinal biochemistry. Schiff base, named by chemist Hugo Schiff, is the structurally diverse compounds in which imine group (-CH=N-) are formed by the condensation of carbonyl and primary amine group. Schiff bases are flexidentate ligands which can stabilize the metal ions in various oxidation states by coordinating them through the lone pair of nitrogen present in azomethine group. The metal



complexes of Schiff base ligands are the centre of attention in the field of bio-inorganic chemistry due to their enhanced pharmacological properties as well as their versatile bonding characteristics. Herein, the design and synthesis of Schiff base ligands have been done and their characterization by spectroscopic techniques such as elemental analysis, IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR and mass spectroscopy. The metal complexes have been synthesized by the reaction of Schiff base ligands with Co(II), Ni(II), Cu(II) and Zn(II) metal salts. All the metal complexes were characterized by elemental analysis, molar conductance, UV-visible spectra, IR, and EPR spectra. TGA has been done to check the stability of the synthesized Schiff base ligands and its metal complexes. On the basis of spectral data, the geometries of metal complexes have been assigned and optimized by using Gaussian 09W software. The DNA/BSA binding studies of metal complexes have been investigated by UV absorbance, fluorescence and CD spectrometry. It has been seen that metal complexes could bind to biomolecules significantly. This property of Schiff base and their metal complexes might be employed in the development of drug design based on the moiety and interactions with various biomolecules, which may further facilitate the discovery of novel and more efficient drugs for various challenging diseases.

#### *Contents*

1. Introduction 2. Synthesis and characterization of Schiff base ligands 3. Synthesis, spectral characterization, and DNA binding studies of Co(II), Ni(II) and Zn(II) complexes of Schiff base ligand HL1 4. Synthesis, spectral characterization, and BSA binding studies of Co(II), Ni(II), Cu(II) complexes of Schiff base ligand HL2 5. Synthesis, spectroscopic characterization and DNA binding studies of metal complexes of Schiff base ligand L3 6. Synthesis, spectroscopic characterization and BSA binding studies of metal complexes of Schiff base ligand HL4 7. Conclusion. Bibliography and Publications.

#### 12. DURGESH KUMAR

#### **Oxazolidine based nsP3 Protease of CHIKV Inhibitor: Designing, Virtual Screening, Docking and Molecular Dynamics Simulations.**

Supervisor: Dr. Prashant Singh

Th 24918

#### *Abstract (Verified)*

Chikungunya fever (CHIKF) is a viral infection, caused by the Chikungunya virus (CHIKV). They are transmitted to humans through the bite of mosquito species like *Aedes aegypti* and *Aedes albopictus*. Non-structural polyproteins consist of four proteins (nsP1-nsP4) and the structural polyproteins consist of five proteins (Capsid (C), E3, E2, 6K and E1). The aim of the thesis is to find the potential candidate to inhibit the activity of nsP3 protease of CHIKV. The nsp3 of CHIKV is essential for minus-strand RNAs and subgenomic 26S mRNAs synthesis and its comparison with the reported molecules. In order to control activity of CHIKV, five multicomponent reaction (MCRs) are designed. The mechanism of chemical reaction was studied through DFT method. Then, a library based on product obtained via MCRs was created and then screened against nsP3 protease of CHIKV. The screened molecule was further screened by biological activity score. Then top five molecules for docking and MD simulation were selected. It is focused on drug-target interactions using various molecular modeling methods, including molecular docking, molecular dynamics (MD) simulations, MM-GBSA (Molecular Mechanics-Generalized Born Surface Area) methods and non-isothermally molecular dynamics simulations.

Change in free energy for the formation of drugs-target complexes are calculated. Visualization of molecular interactions of newly formed drug-target complex system were observed using discovery studio (DS) Visualizer, Pymol, Chimera and molegro molecular viewer (MMV). In this thesis, designing and screening of the designed molecules against nsP3 protease of CHIKV was performed and the candidate, A200 molecules showed best interactions with best binding affinity and minimum  $\Delta G$ . A200 has only one violation for Lipinski's rule of five and bioactivity properties while Baicalin have two violations.

### *Contents*

1. Review of literature 2. Objective of thesis 3. Designing of one pot synthesis get potential molecules and study their mechanism through DFT 4. Design libraries, screening and docking against nsP3 protease of CHIKV 5. DFT, MD simulation and MM-GBSA of top five screened molecules 6. Non-isothermally MD simulations of top one molecule .Summary

13. GARKOTI (Charu)  
**Design and Development of Ionic Liquid Based Heterogeneous Catalysts for Organic Transformations.**  
 Supervisor: Prof. Subho Mozumdar  
Th 24410

### *Abstract* *(Not Verified)*

Right from the discovery of ionic liquids (ILs), they have attained tremendous attention as they are cost effective and environment friendly in nature. It is because of several advantages associated with the usage of ILs, such as low vapor pressure, high thermal and chemical stability, low volatility, high catalytic activity, etc., they have been widely explored in the field of electrochemistry, medicinal chemistry, environment science and catalysis in particular. Although ILs acquire numerous advantages but when used as homogeneous catalysts they are found to have several drawbacks like high viscosity, poor recoverability and difficulty in product purification. In order to address these issues, a concept of heterogenization of ILs using solid support material is being exploited. Various kinds of solid support materials are available, such as carbon, silica and alumina. Following functionalization, the heterogenized IL system can display combined advantages of the solid support material along with that of IL. This thesis work highlights the design and development of several ionic liquid based heterogenous catalyst system and their efficient use as heterogeneous catalysts for various organic transformations. As a whole, this thesis is divided into seven chapters. Chapter 1 provides information about ILs, their utilization as homogenous catalysts and then deals with the elaborated review of the literature on some of the heterogenized IL systems. Chapter 2 briefly discusses the operation principals, working and technical details of all the characterization techniques that have been used in characterizing all the prepared materials presented in this thesis. The next four chapters revolve around the design and development of different ILs and their immobilization over various solid support materials. These chapters include the application and benefits of the prepared materials over others reported in organic transformation reactions. The last chapter (Chapter 7) concludes the current work and also discusses about the future work.

*Contents*

1. Introduction and review of literature 2. Characterization techniques 3. Silica coated magnetic nanoparticles ( $\text{Fe}_3\text{O}_4@\text{SiO}_2$ ) supported imidazolium based ionic liquid : an efficient heterogeneous catalyst for N-formylation of amines. 4. Magnetic core-shell fibrous silica nanospheres supported acetate-based ionic liquid: an efficient and recyclable catalyst for knoevenagel condensation reaction 5. Graphene oxide supported amine-functionalized ionic liquid: an efficient catalyst for the synthesis of 3-substituted indoles via yonemistu-type reaction 6. Magnetic graphene oxide supported amine-functionalized ionic liquid: an efficient catalyst for the synthesis of 3-amino alkylated indoles via mannich-type reaction 7. Conclusion. List of publications.

14. GUPTA (Pankaj)  
**Studies on Multifunctional Inorganic Materials: Selected Examples from Layered Double Hydroxide, Metal Borates, Spinel Structured Oxides and Derivative of Polyaniline.**  
 Supervisor: Prof. Rajamani Nagarajan  
Th 24403

*Abstract*  
 (Not Verified)

Chapter 1 briefly summarized the background literature of layered compounds, metal borate, spinel structured oxides and poly-m-chloroaniline. As short introduction of various structure has been included. Chapter 2 deals with the synthesis and characterization of ethylene glycol intercalated monometallic iron based layered double hydroxide system. Catalytic oxidation and reduction have been done. It could be used for the MRI contrast agent. Chapter 3 deals with the synthesis of vaterite borate system. Transition metal has been doped in  $\text{YBO}_3$ . The optical, photoluminescence and temperature dependent magnetic measurements have been carried out. Ferroelectric, dielectric at room temperature and photocatalytic properties have also been measured. In second part, rare earth has been doped in  $\text{Y}_{0.5}\text{Gd}_{0.5}\text{BO}_3$  system. Photoluminescence study has been done and the symmetric of the doped ions were determined from J-O analysis. Last part was deals with the  $\text{Ce}^{3+}$  doped  $\text{Y}_{0.5}\text{Gd}_{0.5}\text{BO}_3$  and further co-doped with  $\text{Li}^+$ ,  $\text{Ca}^{2+}$  and  $\text{Al}^{3+}$ . The photoluminescence property of  $\text{Ce}^{3+}$  increased with  $\text{Ce}^{3+}$  content, same behaviour was observed in photocatalytic study and it was further improved by co-doping. Chapter 4, section 4.1, deals with the synthesis of non-stoichiometric  $\text{CdGa}_2\text{O}_4$  and substituted by  $\text{Li}^+$  ion. Raman spectra confirmed the purity of the structure. Dielectric properties has been measured for pure and substituted sample. The oxygen ion conductivity as well as photocatalytic activity have been improved by substitution of lithium ion. Section 4.2, deals with the synthesis of pure and  $\text{Cd}^{2+}$  substituted  $\text{ZnAl}_2\text{O}_4$ . Dielectric, ferroelectric, oxygen ion conductivity have been done for  $\text{Cd}^{2+}$  substituted samples. Chapter 5 deals with the synthesis of poly-m-chloroaniline. Adsorption of various carcinogenic dyes have been reported in the thesis. Reduction of aromatic nitro compound has also been done. Chapter 6, The overall conclusions emerged from the present set of investigations summarized in this chapter. Additionally, its implications for futuristic applications to mankind are elaborated.

*Contents*

1. Introduction: Background of the study 2. Ethylene glycol intercalated monometallic layered double hydroxide based on iron as an efficient bifunctional

catalyst 3. Application of epoxide gel synthesis of  $\text{YBO}_3$ , transition metal (Mn & Fe) doped  $\text{YBO}_3$  and rare earth doped  $\text{Y}_{0.50}\text{Gd}_{0.50}\text{BO}_3$  4. Investigation on spinel oxides 5. Adsorption of harmful and carcinogenic organics ordered by semi-crystalline poly-m-chloroaniline (PmCIA) 6. Conclusion and future direction.

15. JAIN (Harshita)  
**Synthesis of N-Heterocyclic scaffolds for colorimetric recognition of ions and Cu (II)-pyridyl complex for degradation of toxic organic dyes.**  
 Supervisor: Dr. Rakesh Kumar  
Th 24384

*Abstract*  
 (Not Verified)

The development of colorimetric chemosensors for recognition of cations and anions is a challenging and emerging area of research due to their harmful/vital roles in biological processes and environment science. We have developed N-Heterocyclic scaffolds for colorimetric recognition of cations and anions. Pyridine-dicarbohydrazide based colorimetric chemosensors has been synthesized for the recognition of  $\text{Cu}^{2+}$ ,  $\text{AMP}^{2-}$ ,  $\text{F}^-$  and  $\text{AcO}^-$  ions. The binding mode of ions is analysed by UV-Vis and  $^1\text{H}$  NMR studies, which is supported by density functional theoretical (DFT) studies. The potential utility of chemosensor has been explored for detection of fluoride ion in commercially available toothpaste. Cu (II)-pyridyl complex CP1, based on (E)-bis-N,N'-(benzo[d]thiazol-2-yl-methylene) pyridine-2,6-dicarbohydrazide ligand has also been synthesized and applied for adsorption as well as photocatalytic degradation of Methylene Blue (MB) and Rhodamine B (RhB) dyes. Seventeen triazole-appended pyrano[2,3-c]pyrazolone based scaffolds have been synthesized out of which, two colorimetric chemosensors has been utilized for the "cascade recognition" of  $\text{Fe}^{3+}$  and  $\text{H}_2\text{PO}_4^-$  ions. Metal-chemosensor ensemble was found to respond to  $\text{H}_2\text{PO}_4^-$  ions out of all other anions. The colorimetric response was utilized to develop "INHIBIT" logic gate. These chemosensors were also applied to detect  $\text{Fe}^{3+}$  ion in real samples such as blood sample and tap water. Three new triazole-appended isatin based colorimetric sensors has been synthesized by Cu (I) catalysed azide-alkene cycloaddition reaction for recognition of  $\text{Fe}^{3+}$  ion. The chemosensors exhibited excellent selectivity for  $\text{Fe}^{3+}$  ions in presence of competitive metal ions. The selectivity and sensitivity of all the chemosensors was investigated through colorimetric and UV-Vis studies. The limit of detection (LOD) of chemosensor for binding of  $\text{Fe}^{3+}$  and  $\text{Cu}^{2+}$  ions were determined to be much lower than the value recommended by US Environmental Protection agency.

*Contents*

1. Synthesis of highly sensitive pyridine-dicarbohydrazide based chemosensor for colorimetric recognition of  $\text{Cu}^{2+}$ ,  $\text{AMP}^{2-}$ ,  $\text{F}^-$  and  $\text{AcO}^-$  ions 2. Synthesis of highly efficient multifunctional Cu (II)-pyridyl complex for adsorption and photocatalytic degradation of organic dyes 3(A). Metal catalyzed synthesis of pyranopyrazole and triazole-appended pyrano[2,3-c]pyrazolone scaffolds 3(B). Triazole-appended pyrano[2,3-c]pyrazolone based colorimetric chemosensors for recognition of  $\text{Fe}^{3+}$  ions and their molecular logic gate behaviour 4. Isatin-triazole tethered tetrahydropyridine based sensors for selective recognition of  $\text{Fe}^{3+}$  ion. Summary and published paper.

16. KANDI (Shamseer Kulangara)  
**Strategic Design, Synthesis, and Bio-Evaluation of Molecular Hybrids as Possible Therapeutics**  
 Supervisor: Prof. Diwan S. Rawat  
Th 24405

*Abstract*  
 (Not Verified)

This work is aimed towards developing novel drug molecules against fatal diseases that afflict human lives. Malaria is one such deadly infectious disease that mainly affects economically poor nations. The development of resistance against cheaply available antimalarial drug chloroquine (CQ) and the alternate drug, artemisinin (ART) is raising serious concern. To overcome this problem, chemical modification of antimalarial drugs and the hybridization of antimalarials with other pharmacophores are widely appreciated approaches. Hybridization is a method where two or more biologically active pharmacophores are covalently linked, in anticipation to improve the biological activity and overcome drug resistance. Based on these approaches, in chapters 1 and 2, the antimalarial drug chloroquine was modified by the hybridization of quinazoline with pyrimidine moiety. This led to the synthesis of 96 novel 4-aminoquinazoline-quinazoline and 4-aminoquinoline-pyrimidine hybrids. In the first series, 20 compounds have shown better antimalarial activity against CQ sensitive strains compared to the reference drug CQ and ART. Interestingly, 38 compounds have shown better antimalarial activity against CQ resistant strains than the reference drug CQ and the in-vivo screening of selected 4 compounds are under progress. In chapter 2, the preliminary results showed that the hybrids were better active over the reference drug CQ against both resistant and sensitive strains. In chapter 3, an antimalarial and promising anti-Parkinson drug amodiaquine was modified by hybridizing it with pyrimidine pharmacophores, and it resulted in compounds having better antimalarial and anti-Parkinson activities. In continuation, to further improve the anti-Parkinson activity, 4-anilinoquinazoline-pyrimidine hybrids were synthesized and the studies are under progress. Similarly, in chapter 4A, the 4-aminoquinoline pharmacophores were hybridized with C5-curcumin that imparted promising antitumor activity. In chapter 4B, novel tri-substituted pyrimidines were investigated for improved antimycobacterial activity. Overall, more than 170 novel molecules have been synthesized with promising biological activity.

*Contents*

1. Strategic design, synthesis characterization, and bio-evaluation of 4-aminoquinoline-quinazoline hybrids as antimalarial and anticancer agents 2. An investigation of 4-aminoquinoline-diphenyl substituted pyrimidine hybrids as antimalarial and antiviral agents 3. Synthesis and bio-evaluation of modified amodiaquine/4-anilinoquinazoline-pyrimidine hybrids as antimalarial and anti-parkinson agents 4(A). C5-curcuminoid-4-aminoquinoline based molecular hybrids: design, synthesis, and mechanistic investigation of anticancer activity 4(B). Synthesis and biological evaluation of tri-substituted pyrimidines as anti-infective agents. Summary and list of publications and patents.

17. KAUR (Harsimran)  
**Some Aspects of Neutral and Charged Exciton Complexes of 2-D and 3-D Anisotropic Quantum Dots and Transition Metal Dichalcogenides in Magnetic Field by Exact Multipole Expansion of Coulomb Interactions.**  
 Supervisor: Prof. Ram Kuntal Harza  
Th 24391

*Abstract*  
(Not Verified)

Chapter-1 - A comprehensive literature survey of quantum dots, excitons, fabrication techniques of quantum dots, Transition Metal Dichalcogenides and concise summary of the essentials of various electronic structure calculations and indispensable mathematical tools and techniques involved in the theoretical development of the formalism in the thesis have been described. Chapter-2 - A rigorous mathematical formalism outlining an exact variational approach to coulomb (exchange) interactions between a pair of electron and hole, i.e., exciton within a 2-D quantum dot is presented. Chapter-3 - A specific and comparative study of the electronic structure and inferences drawn from the same have been documented in detail. Chapter-4 - The study of level spacing statistics and thermodynamic properties such as Specific Heat and Magnetization at different confinement frequencies and system parameters for He, SiO<sub>2</sub>, BN and GaAs model systems has been discussed. Chapter-5- An exact variational treatment for multi-dynamic attracting and scattering interactions among neutral and charged N-excitonic complexes (N= 2,3,4,...) in presence of anisotropy by use of Lauricella function and Chu-vandermonde identity has been achieved. Chapter-6 - The effect of anisotropy in destroying Fock-Darwin spectra exhibited by non-interacting isotropic N-excitonic complexes in TMDCs/QDs has been investigated. Chapter-7 - Binding energy of neutral and charged multi-excitonic complexes for TMDCs have been evaluated in zero and non-zero magnetic field. Chapter-8 - Properties such as Chemical potential and addition energy spectra have been investigated. The addition energy spectra of N-excitonic complexes in TMDCs/QDs exhibit a fingerprint shell structure. Chapter-9 - A generalized approach analyzing the dynamics of charged 'N'-excitonic systems of TMDCs/3-D anisotropic quantum dots in presence of arbitrary magnetic field via multipole expansion of coulomb interactions taking into account anisotropy inherent in system is presented. Chapter-10 - The electronic structure and role of anisotropy in exciton complexes in 3-D anisotropic quantum dots/TMDCs has been investigated.

*Contents*

1. Introduction 2. Extract theoretical development of an excitonic (e-h) system in 2-D quantum dots 3. Electronic structures of 2-D excitonic systems 4. Level spacing statistics, specific heat ( $C_v$ ) and magnetization (M) 5. Exact formalism of neutral and charged exciton complexes of 2-D anisotropic quantum dots/transition metal dichalcogenides 6. Electronic structures of exciton complexes of 2-D anisotropic quantum dots/transition metal dichalcogenides 7. Elucidation of binding energy of neutral and charged exciton complexes of 2-D anisotropic quantum dots/transition metal dichalcogenides 8. Chemical potential and addition energy spectra of 2-D exciton complexes 9. Formalism of neutral and charged exciton complexes of 3-D anisotropic quantum dots/transition metal dichalcogenides 10. Electronic structures of 3-D anisotropic exciton complexes. .Summary and future perspectives .Bibliography and list of publications.

18. KHURANA (Ishani)  
**Synthesis, characterization and applications of graphene based materials for purification of water and synthesis of heterocycles.**  
 Supervisors: Prof. J. M. Khurana and Dr. P. K. Rai  
Th 24388

*Abstract*  
(Not Verified)

This thesis entitled “Synthesis, characterization and applications of graphene based materials for purification of water and synthesis of heterocycles” presents synthesis and applications of graphene-based materials. The subject matter of the thesis is divided into VI chapters. Each chapter is subdivided into four sections (1) Introduction, (2) Results and Discussion, (3) Experimental and (4) References. The Results and Discussion in Chapter II and VI has been subdivided in two parts. The chapter wise brief account is given below. Chapter I describes synthesis and characterization of nano  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> impregnated reduced graphene oxide sheets ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>-rGO).  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>-rGO has been applied for the adsorptive removal of 2,4,6-trinitrophenol (TNP) from water. Chapter II is divided in two parts. In Part A, water contaminated with Eriochrome Black T (EBT) has been purified using  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>-rGO. In Part B of this chapter,  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>-rGO has been utilized for the removal of TNT (2,4,6-trinitrotoluene) from aqueous solutions. In Chapter III, nano zero valent iron loaded on rGO sheets (nZVI-rGO) has been synthesized and characterized. nZVI-rGO has been utilized for the removal of TNT from water. Adsorptive removal of RDX (Royal Demolition eXplosive) and HMX (High Melting eXplosive) from water using  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>-rGO and nZVI-rGO as adsorbents has been reported in Chapter IV. Synthesis of 1,3-oxazines derivatives by condensation of aromatic/aliphatic amines, formaldehyde and sesamol/2-hydroxy-1,4-naphthoquinone/6-hydroxyquinoline in aqueous medium at room temperature using rGO as the catalyst forms the subject matter of Chapter V. Chapter VI has been divided into two parts. Part A describes an efficient synthesis of novel benzo[d]imidazo[2,1-b]thiazoles from 2-aminobenzothiazole, phenylglyoxals and cyclic enolisable 1,3-dicarbonyl compounds in water catalyzed by rGO under ultrasonic radiations at room temperature. Part B reports application of 4-hydroxy-6-methyl-3-(2-phenylbenzo[d]imidazo[2,1-b]thiazol-3-yl)-2H-pyran-2-one as a selective probe for the detection of Pb<sup>2+</sup> and Al<sup>3+</sup> ions. Chapter VII is a summary and conclusions of the work reported in this thesis.

*Contents*

1. Synthesis, characterization and application of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>-rGO for the removal of 2,4,6-trinitrophenol (TNP) from water  
 2. Application of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>-rGO for the removal of eriochrome black T (EBT) and 2,4,6-trinitrotoluene (TNT) from water  
 3. Synthesis, characterization and application of nZVI-rGO for the removal of 2,4,6-trinitrotoluene (TNT) from water  
 4. Application of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>-rGO and nZVI-rGO for the removal of 1,3,5-trinitro-1,3,5-triazinane (RDX) and 1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX) from water  
 5. rGO mediated synthesis of various 1,3-oxazine derivatives in aqueous medium  
 6. Synthesis of benzo[d]imidazo[2,1-b]thiazole derivatives and their application for detection of Al<sup>3+</sup> and Pb<sup>2+</sup> ions  
 7. Summary, conclusions and list of publications.

19. MANDEEP  
**DFT Study on Graphene-based Adsorbents for Water Remediation.**  
 Supervisor: Prof. Reeta Kakkar  
Th 24401

*Abstract*  
(Verified)

The aim of the research work presented in this thesis is to study modified graphene-based surfaces for the efficient removal of pollutants from water systems. Harmful organic pollutants like aromatic compounds, pesticides and dyes cause various

health hazards among living beings. Therefore, pre-discharge treatment of wastewater is of paramount importance. The conventional water treatment methods such as distillation, reverse osmosis and coagulation-flocculation are less effective and cumbersome. In this regard, adsorption is a method of choice due to its effectiveness, ease of operation and low cost. Graphene is an apt surface due to its whole volume, i.e., all carbon atoms are exposed to the analyte of interest due to its two-dimensional structure. The strong mechanical properties of graphene, high surface area and excellent thermal conductivity are highly favorable for various applications. Graphene can also be modified by doping and creating defects. Hence, the structural modifications by creating vacancies or doping metal atoms can alter the electronic properties and reactivity of graphene. On doping a transition metal atom on a graphene sheet the reactivity of the graphene sheet increases. Moreover, the lamellar structure provides sites for doping other nanoparticles to create nanocomposites for enhancing the adsorption capacity and facilitating separation from the solutions. In this work, we have performed DFT study by taking various hazardous pollutants like bromonitromethane, para-nitrophenol and pesticides such as carbaryl and glyphosate and have studied their adsorption on modified graphene surfaces. We found that pristine graphene shows physisorption for these pollutants while modified graphene exhibits chemisorption. Thus graphene based adsorbents are suitable candidate for adsorptive removal of such pollutants.

#### *Contents*

1. Graphene-based adsorbents for water remediation by removal of organic pollutants: theoretical and experimental insights 2. Computational techniques 3. Adsorption of bromonitromethane on graphene-based substrates: a density functional theory analysis 4. DFT Study on the adsorption of p-nitrophenol over vacancy and Pt-doped graphene sheets 5. DFT study of carbaryl pesticide adsorption on mono vacancy graphene and nitrogen doped graphene decorated with platinum clusters 6. DFT study of adsorption of glyphosate pesticide on Pt-Cu decorated pyridine-like nitrogen doped graphene 7. Conclusions and perspectives, appendices and bibliography.

20. MANISH KUMAR

**Optical and Electrical Properties of Few Oxide Systems Possessing Fluorite and Spinel Structure Prepared by Wet Chemical Methods.**

Supervisor: Prof. Rajamani Nagarajan

Th 24917

#### *Abstract* (Not Verified)

A general introduction to various aspects of materials chemistry in today's scenario has been outlined in chapter 1. Chapter 2 has been divided in to five subsections. To address the existing gap in the literature of upconversion studies involving thoria, samples of thoria doped with Ho<sup>3+</sup>: Yb<sup>3+</sup>, Er<sup>3+</sup>: Yb<sup>3+</sup>, and Tm<sup>3+</sup>: Yb<sup>3+</sup> were synthesized following epoxide gel method and were characterized. The results along with discussion of them have been included in section 2.1. Section 2.2 deals with studies involving the incorporation of some divalent transition-metal ions in thoria and to comprehend its effect on the crystal, electronic structures as well as catalytic properties. Ni<sup>2+</sup>, Cu<sup>2+</sup> and Cd<sup>2+</sup> substituted thoria samples were synthesized by the epoxide gel method. In section 2.3, our attempts to modulate the anionic defects in the thoria system by co doping nickel and copper along with yttrium have been discussed. Section 2.4 describes the outcome of incorporation of lead in fluorite structured thoria in terms of structure and electrical properties. Samples with



stoichiometries  $\text{Th}_{1-x}\text{Pb}_x\text{O}_{2-\delta}$  ( $x = 0.00$  to  $0.70$ ) have been synthesized by a solution combustion route and characterized extensively. Similar investigation has been extended to ceria system where in lead substitution was found to be successful up to 50 mol % retaining fluorite structure. The results along with discussion of them have been included in section 2.5. Chapter 3 deals with our efforts to include spectroscopically rich  $\text{Eu}^{3+}$  and  $\text{Tb}^{3+}$  in non-stoichiometric  $\text{CdGa}_2\text{O}_4$  and examine their luminescence properties. Synthesis and characterization of red emitting  $\text{Cr}^{3+}$  containing cadmium gallate has also been included. The overall conclusions drawn from these investigations together with scope for further studies have been elaborated in chapter 4.

#### *Contents*

1. Introduction 2. Work on fluorite structured thoria and ceria 3. Optical, magnetic property and photocatalytic evaluations of rare-earth ( $\text{Eu}^{3+}$ ,  $\text{Tb}^{3+}$ ) and  $\text{Cr}^{3+}$  substituted gallium rich cadmium gallate 4. Conclusions and future directions .List of publications.

21. MEENAKSHI  
**Development of Metal Chalcogenide and Alloy Nanostructured Catalysts for Electrocatalytic and Photocatalytic Water Spitting Reaction.**  
 Supervisor: Dr. Sasanka Deka  
Th 24920

#### *Contents*

1. Introduction 2. Synthetic approaches and experimental details 3. Development of 2-dimensional copper cobalt sulphide nanosheets realizing a promising electrocatalytic for efficient water oxidation 4. A promising visible-light driven hydrogen production from water on highly efficient  $\text{CuCo}_2\text{S}_4$  nanosheets photocatalyst 5. Cobalt sulphide hollow nanoparticles: a robust and lost cost universal pH responsive oxygen evolution as well as overall water splitting electrocatalyst 6. High performing dealloyed or leached  $\text{AfNi}$  alloy nanoparticles as an efficient electro-catalyst for hydrogen evolution reactions .Summary and list of publications.

22. MITTAL (Anshika)  
**In silico studies of inducible nitric oxide synthase inhibitors.**  
 Supervisor: Prof. Rita Kakkar  
Th 24406

#### *Abstract* *(Verified)*

Inducible nitric oxide synthase (iNOS), which catalyzes the synthesis of nitric oxide (NO) in mammals, that in turn acts as a cytotoxic agent in the immune system, has also been found to be associated with various pathological conditions and disorders, when NO is produced by iNOS in excess. Therefore, inhibition of iNOS activity provides an important therapeutic approach to the design of new drugs that target iNOS. Computational techniques have also been applied to develop novel drugs and to get a better insight and understanding into the structural basis of the potency and selectivity of iNOS-specific inhibitors. In this work, in silico studies have been performed on iNOS inhibitors in order to get a better insight into the binding of these inhibitors, and propose novel iNOS inhibitors. Aminopyridines and quinazolines, which have earlier been reported as highly potent and selective inhibitors of iNOS

that bind into its active site through the anchored plasticity approach, have been investigated by pharmacophore modeling and 3D-QSAR studies. Novel iNOS drugs have also been proposed by using pharmacophore-based virtual screening. Docking studies have also been performed on some iNOS inhibitors in order to study the effect that different substituents have on the potency and selectivity of these inhibitors. Induced fit docking studies have also been done in order to investigate the changes that occur in the protein conformation on binding of the inhibitors. Overall, our studies have provided valuable and important information on binding of these iNOS inhibitors, which is expected to prove useful for further investigations on iNOS inhibitors, and develop novel and more potent and selective inhibitors of iNOS.

### Contents

1. Nitric oxide synthases and their inhibitors: A review 2. Computational techniques 3. Pharmacophore modelling and 3D-QSAR studies of quinazolines and aminopyridines as selective inhibitors of inducible nitric oxide synthase 4. Identification of novel potent and selective inducible nitric oxide synthase inhibitors: virtual screening and molecular docking studies 5. In *silico* study of the inhibition of inducible nitric oxide synthase by spirocyclic quinazolinamines 6. Induced fit docking of non-amidine inhibitors of inducible nitric oxide synthase 7. Concluding remarks and Bibliography.

23. MOHIT

**Development of methodologies for the synthesis of novel N/O/S containing heterocycles, photophysical properties and application of nickel boride.**

Supervisor: Prof. Ramesh Chandra

Th 24400

*Abstract*  
(Not Verified)

This thesis entitled "Development of methodologies for the synthesis of novel N/O/S containing heterocycles, photophysical properties and application of nickel boride" presents some novel synthetic methods, which include seven chapters and each chapter I to VII has been subdivided into sections (1) Introduction, (2) Results and Discussion, (3) Experimental and (4) References. The chapter wise brief account is given below. Chapter I describes catalyst free synthesis of novel 5-substituted 6-phenylpyrrolo[2,3-d]pyrimidines by one-pot three component condensation of 6-amino-1,3-dimethyluracil, phenylglyoxal with indoles/active methylene compounds in ethanol at reflux temperature. Chapter II has reported triphenylphosphine mediated synthesis of novel fumarate substituted 3-acylcoumarins by reaction of 3-acylcoumarins and dialkyl acetylenedicarboxylates in THF at room temperature and the structure of a compound was also confirmed by X-Ray analysis. Chapter III describes the synthesis of novel naphtho[1,2-e][1,3]thiazines, naphtho[2,1-e][1,3]thiazines and benzo[e][1,3]thiazines by one-pot three component condensation of amines and formaldehyde with 2-thionaphthol/1-thionaphthol/substituted thiophenols in presence of TBAB at 100 oC under solvent free conditions. Acetic acid mediated sequential one-pot multicomponent reaction of aldehydes/ketones, thiosemicarbazide, arylglyoxal and active methylene compounds for the synthesis of 2,4,5-trisubstituted thiazoles in ethanol at reflux temperature has been described in Chapter IV. K<sub>2</sub>CO<sub>3</sub> mediated thioarylation, selenoarylation and arylation of 2-aminomaleimides by reaction with thiophenols, diarylbiselenides and phenyl hydrazines, respectively in DMSO at room temperature has been described in Chapter V and X-Ray analysis of a thioarylated and arylated product has also been discussed. Chapter VI reports the synthesis of a novel thionoxanthene, 9,9-dimethyl-

12-(4-(prop-2-yn-1-yloxy)phenyl)-9,10-dihydro-8H-benzo[a]xanthene-11(12H)-thione (1) and its application as a colorimetric sensor for selective detection of Hg (II). Chapter VII includes the deprotection of benzyloxycarbonyl (Cbz) protected amines/phenols to the corresponding amines/phenols with nickel boride, generated in situ from nickel chloride and sodium borohydride, in methanol at ambient temperature. Chapter VIII is a summary and conclusions of the work reported in this thesis.

### Contents

1. Catalyst free synthesis of novel 5-substituted 6-phenyl pyrrolo[2,3-*d*]pyrimidines by one-pot three component reaction 2. Triphenylphosphine mediated stereoselective synthesis of fumarate substituted 3-acylcoumarins 3. TBAB mediated synthesis of novel naphtho[1,2-*e*] [1,3]thiazines, naphthos[2,1-*e*][1,3]thiazines and benzo[*e*][1,3]thiazines 4. Acetic acid mediated regioselective synthesis of 2,4,5-trisubstituted thiazoles by domino reaction 5.  $K_2CO_3$  mediated thioarylation, selenoarylation and arylation of 2-aminomaleimides 6. Synthesis and application of 11-thionoxanthene derivative as a colorimetric sensor for selective detection of Hg (II) 7. Nickel boride mediated chemoselective deprotection of N/O-benzyloxycarbonyl (Cbz) compounds 8. Summary, conclusions and list of publications

24. NEELAM  
**Iron Oxide Based Multifunctional Nanoparticles for Biomedical/ Environmental Applications.**  
 Supervisor: Dr. Mahima Kaushik  
Th 24385

### Abstract (Not Verified)

In nano-biotechnology field, biocompatible materials comprising of DNA and magnetic nanoparticles (MNPs) in combination have recently attracted lot of attention. Understanding of these systems is extremely important for the development of areas especially like biomedical diagnosis and treatment (development of sensitive biosensors and effective pharmaceuticals) of various diseases. The combination of MNPs with biological molecules and especially nucleic acids allow the development of various hybrid nano-systems having unique magnetic properties and biological selectivity. Spinel ferrites ( $MFe_2O_4$ ,  $M = Zn, Ni, Co, Mn$ ) are one of the most important magnetic nanomaterials because of their rich electronic, magnetic, dielectric, optical and catalytic properties which strongly depend on the distribution of cation in tetrahedral and octahedral sites, where a synergism exist between  $Zn^{2+}$  and  $Fe^{3+}$  ions. Therefore, synthesis of these magnetic nanomaterials and utilization of their excellent properties for biomolecules interaction makes them peculiar candidates for biomedical applications. Silica coated  $Fe_3O_4$  and  $ZnFe_2O_4$  nanoparticles have good biocompatibility, therefore amino-propyl-triethoxy silane (APTS) molecule is used as silica and amine ( $-NH_2$ ) source in this study. Firstly, we had synthesized  $Fe_3O_4$  and  $ZnFe_2O_4$  nanoparticles with amine composite particles via single/ one pot hydrothermal method. Further, the interaction of these functionalized nanoparticles with nucleic acid (DNA) and protein (bovine serum albumin; BSA) was investigated based on various physicochemical and biophysical techniques for exploring their biomedical applications. Also, due to increase in urbanization and industries, discharge of hazardous contaminants in the form of organic dyes from various industries like textile, dyeing and other related processes enormously pollute the water resources and cause adverse impacts on the environment and human health. Therefore, application of thus synthesized  $ZnFe_2O_4$

and APTS coated ZnFe<sub>2</sub>O<sub>4</sub> nanoparticles were further explored for the degradation of dyes like acridine orange and proflavine.

### Contents

1. Introduction to iron oxide based multifunctional nanoparticles and their biomedical/ environmental application 2. Techniques for characterization of nanoparticles and to study interaction with biomolecules 3. Synthesis, characterization and interaction of magnetite and 3-aminopropyl triethoxy silane (APTS) coated magnetite nanoparticles with calf thymus DNA (Ct-DNA) 4. Synthesis, characterization and interaction of zinc ferrite (ZnFe<sub>2</sub>O<sub>4</sub>) and 3-aminopropyl triethoxy silane (APTS) coated zinc ferrite nanoparticles with calf thymus DNA (Ct-DNA) 5. Synthesis, characterization and interaction of zinc ferrite (ZnFe<sub>2</sub>O<sub>4</sub>) and 3-aminopropyl triethoxy silane (APTS) coated zinc ferrite (ZnFe<sub>2</sub>O<sub>4</sub>) nanoparticles with bovine serum albumin (BSA) protein 6. A comparative study of textile and biological dye degradation using ZnFe<sub>2</sub>O<sub>4</sub> and APTS-ZnFe<sub>2</sub>O<sub>4</sub> photo catalysts under solar and artificial visible light 7. Conclusions, bibliography and list of publications.

25. PANDEY (Stuti)  
**Synthesis of Novel Bis-Benzthiazoles/Bis-Benzimidazoles and their Evaluation as Anticancer and Antibacterial Agent.**

Supervisors: Prof. Akhilesh Kumar Verma and Prof. Vibha Tandon  
 Th 24394

### Abstract (Not Verified)

The thesis includes the synthesis of Bis-benzothiazoles analogues. We synthesized 18 novel benzimidazole analogues. The other part of the study includes DNA binding study of substituent specific Bis- benzimidazole analog for understanding drug-DNA interaction. On binding to DNA, fluorophore exhibits a substantial amount of fluorescence enhancement because of the loss of solvent exposure on snugly binding (van der Waals and H-bonding forces) inside the DNA groove. There is a remarkable increase in fluorescence of ligands upon binding to the duplex at drug/oligomer ratio,  $r = 0.2:1$ . We determined their binding affinity with oligomeric duplex by Scatchard plots here too and the stoichiometries found to be around 1 which validated our absorption-titrations. All 18 synthesized compounds were evaluated for their cytotoxicity by using MTT against seven different cancerous cell line (a) human lung adenocarcinoma epithelial (A-549), NIH 3T3 mouse embryonic fibroblast, HeLa cervical cancer cells line. Most of the compounds exhibited cytotoxicity against various cancer cell lines. We subjected the synthesized compounds against six different MDR Gram-negative bacterial species namely Klebsiella spp, Pseudomonas spp, Acinetobacter spp, Shigella spp, Salmonella spp and Escherichia coli and two MDR Gram-positive bacterial species Enterococcus spp and Staphylococcus spp. Two of the synthesized compounds, BPVF and BPEF showed bactericidal activity against a broad range of bacteria. We also studied binding affinity of bisbenzimidazole derivatives having different substitutions on phenyl ring and piperazine nucleus towards AT rich DNA. The results suggest that an increase of chain length at one end bind with a differential affinity towards duplex DNA.

### Contents

1. Review of literature 2. Synthesis of novel heterocyclic molecules 2A. Synthesis of Bis-benzimidazoles derivatives 2B. Synthesis of Bis-benzothiazoles derivatives 3.

DNA binding study of Bis-benzimidazoles derivatives by using UV –spectroscopy and fluorescence spectroscopy 4. Biological evaluation of Bis-benzimidazole and Bis-benzothiazoles 4A. Bis-benzimidazoles and Bis-benzothiazoles as anticancer agents 4B. Bis-benzimidazoles as antibacterial activity .Publications.

26. PUROHIT (Gunjan)

**Target Oriented Synthesis of Nanomaterials: Application in Organic Transformations and Photosensitization.**

Supervisor: Prof. Diwan S. Rawat

Th 24924

*Abstract  
(Not Verified)*

In chapter 1, HS-CuO nanocatalyst was developed to afford benzofuranamine and dihydro-benzofuranamine isomers with anomalous selectivity via O-annulated A3 coupling among salicylaldehydes, secondary amines and alkynes followed by cycloisomerization in the absence of base/solvent. HS-CuO nanocatalyst was recycled for five times and offers several advantages such as wide substrate scope, anomalous selectivity in the products, high yields, short reaction time, avoided the usage of extra reagents and showed ideal values of green chemistry metrics. In chapter 2a and 2b, A sustainable method for the synthesis of substituted pyrrolidines/piperidines was developed by employing CuAl-MO nanocomposites and Cu<sub>2</sub>O@Fe<sub>3</sub>O<sub>4</sub>/C as catalytic systems. Both catalysts were well characterized using various techniques such as HR-XRD, HRTEM, SEM, ICP, BET, XPS etc. The catalysts were recyclable and shows low leaching levels of respective metal ions. In chapter 3a, copper indium ethylxanthate was used as a versatile precursor for synthesis of colloidal chalcopyrite phase copper indium sulphide (CC-CIS NPs) in photosensitization of graphene quantum dots and reusable powdered wurzite phased copper indium sulphide nanoparticles for selective and efficient single pot sustainable synthesis of substituted imidazopyridines via A3 coupling strategy of an aldehyde, amine and alkyne. In chapter 3b, GQDs have been synthesized by an inexpensive facile bottom-up approach i.e. pyrolysis of L-glutamic acid. The results manifested that the synthesized ZnO-GQDs composites could be a potential candidate for photovoltaic applications as well as suitable catalytic system for the synthesis of tetrasubstituted propargylamines. In chapter 4a, Palladium nanoparticles were impregnated on porous silica shell carbon-coated cobalt nanoparticles, resulting in a magnetically retrievable material that was evaluated in the catalytic hydrogenation of nitroarenes, alkenes and alkynes. In chapter 4b, the solvent less coupling of aldehydes (1a – i) and amines (2a - e) in 1:2 (aldehyde : amines) ratio yielded amins, which were thoroughly characterized through <sup>1</sup>H, <sup>13</sup>C NMR confirming structures of resulted products.

*Contents*

1. HS-CuO NPs catalyzed synthesis of benzofuran isomers with anomalous selectivity 2a. CuAl-MO nanocomposites mediated expeditious synthesis of 2-alkynyl-pyrrolidines/piperidines with ideal green chemistry metrics 2b. Magnetically action Cu<sub>2</sub>O@Fe<sub>3</sub>O<sub>4</sub>/C nanocomposites catalyzed synthesis of 2-alkynyl-pyrrolidines/piperidines *via* KA2 reactions 3a. Synthesis and characterization of CuInS<sub>2</sub> based nanocomposites and its application in photosensitization and one pot green synthesis of immedazopyridines derivatives 3b. Design and synthesis of XnO-GQDs NCs: application in photosensitization and KA2 coupling reactions with their ideal green chemistry metrics 4a. Palladium nanocatalysts encapsulated on porous silica @ magnetic carbon-coated cobalt nanoparticles (Pd@Co/C-SiO<sub>2</sub>-NH<sub>2</sub> NPs): an

efficient nanocatalyst for the hydrogenations of nitroarenes and unsaturated C-C bonds 4b. Water catalysed on pot synthesis of animals .Summary and list of publications.

27. RATHI (Garima)  
**Synthesis, Characterization and Applications of Various Layered Double Hydroxides (LDHs).**  
 Supervisor: Prof. Ramesh Chandra  
Th 24921

*Abstract*  
*(Not Verified)*

According to a recent survey by GOES organization, water pollution is considered to be one of the leading environmental problems which can be a threat to life's existence on the planet in the upcoming decades. Therefore, it has become a great concern of various societies. To deal with this problem, the various LDHs have been designed and characterized using various techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy, high-resolution transmission electron microscopy (TEM) and so on. The obtained LDHs and modified forms were further used for the removal of organic contaminants (such as dyes and antibiotics) and heavy metals from wastewater. One of the obtained modified LDHs was also used for catalytic synthesis of xanthenes and 1,4-Dihydropyridine derivatives. This work has been distributed into seven chapters (including- Introduction, Review of Literature and Aims and Objectives).

*Contents*

1. Introduction 2. Review of literature 3. Aim and objectives 4. A new biocompatible ternary layered double hydroxide absorbent for ultrafast removal of anionic organic dyes 5. A catalytic approach for the synthesis of xanthene and 1,4-dihydropyridine derivatives by calcined layered double hydroxide 6. MoS<sub>4</sub><sup>2-</sup> intercalated NiFeTi LDH: an efficient and selective absorbent for elimination of heavy metals 7. Simultaneous elimination of dyes and antibiotic with a hydrothermally generated NiAlTi layered double hydroxide absorbent .Summary and research publications.

28. RAVI KANT  
**Synthesis, Spectral Characterization, Theoretical Studies and Applications of Transition Metal Complexes of Schiff Base Ligands.**  
 Supervisors: Prof. Ramesh Chandra and Dr. Sulekh Chandra  
Th 24413

*Abstract*  
*(Not Verified)*

The metal-based drug has gained much attention due to their wide applications in the field of medicinal biochemistry. Schiff base, named by chemist Hugo Schiff, is the structurally diverse compounds in which imine group (-CH=N-) are formed by the condensation of carbonyl and primary amine group. Schiff bases are flexidentate ligands which can stabilize the metal ions in various oxidation states by coordinating them through the lone pair of nitrogen present in azomethine group. The metal complexes of Schiff base ligands are the centre of attention in the field of bio-inorganic chemistry due to their enhanced pharmacological properties as well as their versatile bonding characteristics. Herein, the design and synthesis of Schiff base ligands have been done and their characterization by spectroscopic techniques

such as elemental analysis, IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR and mass spectroscopy. The metal complexes have been synthesized by the reaction of Schiff base ligands with Co(II), Ni(II), Cu(II) and Zn(II) metal salts. All the metal complexes were characterized by elemental analysis, molar conductance, UV-visible spectra, IR, and EPR spectra. TGA has been done to check the stability of the synthesized Schiff base ligands and its metal complexes. On the basis of spectral data, the geometries of metal complexes have been assigned and optimized by using Gaussian 09W software. The DNA/BSA binding studies of metal complexes have been investigated by UV absorbance, fluorescence and CD spectrometry. It has been seen that metal complexes could bind to biomolecules significantly. This property of Schiff base and their metal complexes might be employed in the development of drug design based on the moiety and interactions with various biomolecules, which may further facilitate the discovery of novel and more efficient drugs for various challenging diseases.

### Contents

1. Introduction: ligands and their transition metal complexes 2. Synthesis and spectroscopic characterization of ligands (L<sup>1</sup>-L<sup>4</sup>) 3. Synthesis and spectroscopic characterization of manganese (II) complexes of ligands (L<sup>1</sup>-L<sup>4</sup>) 4. Synthesis and spectroscopic characterization of cobalt (II) complexes of ligands (L<sup>1</sup>-L<sup>4</sup>) 5. Synthesis and spectroscopic characterization of nickel (II) complexes of ligands (L<sup>1</sup>-L<sup>4</sup>) 6. Synthesis and spectroscopic characterization of copper (II) complexes of ligands (L<sup>1</sup>-L<sup>4</sup>) 7. Screening of biological activities of synthesized compounds antifungal activity and antibacterial activity .List of publication.

29. REETA

#### **Study of Palladium-Catalysed Carbon-Oxygen Cross-Coupling Reactions of Aryl Bromides and Bromochalcones with Oxygen Nucleophiles.**

Supervisors: Dr. R. P. Singh and Dr. Raj Pal Singh

Th 24402

#### *Abstract (Not Verified)*

The thesis entitled “Study of Palladium-Catalysed Carbon-Oxygen Cross-Coupling Reactions of Aryl bromides and Bromochalcones with Oxygen Nucleophiles” to be submitted to University of Delhi. The research work mainly deals with the development of new synthetic methodologies to make C–O bond formation between activated aryl bromides and bromochalcones with oxygen nucleophiles by Pd/phosphine ligand catalyst systems. The oxygen nucleophiles have been chosen to incorporate in the organic molecules by Pd-catalysed method are methanol and higher alkyl alcohols, ethyl acetohydroxamate, ketoximes and aldoximes. The ethers derived from these nucleophiles would be of great interest in pharmaceutical chemistry and in organic synthesis. The novel chalcones have been synthesized for the first time by Pd-catalysed methodology from bromochalcones and different oxygen nucleophiles. The thesis is divided into five chapters. The first chapter begins with a brief introduction of Pd-catalysed cross-coupling reactions and the explored the detailed literature survey of Pd-catalysed C–O cross-coupling reactions. The synthesis of chalcones by novel methodology has also discussed. This also sets the stage for the scope of the work carried out embodied in the current thesis. The second chapter deals with the novel methodology for Pd-catalysed methoxylation and trideuteriomethoxylation of bromochalcones in short reaction time usually 5 min. This methodology may be adopted for the <sup>11</sup>C-radiolabeling of organic compounds for PET imaging applications. The third chapter describes the development of an efficient methodology for Pd-

catalysed C–O cross-coupling of ethyl acetohydroxamate with 4-bromochalcones to synthesize novel chalcones. The fourth chapter deals with an efficient Pd-catalysed methodology for C–O cross-coupling of activated aryl bromides and bromochalcones with ketoximes and chalcone oximes. The fifth chapter deals with a Pd-catalysed C–O cross-coupling of aryl bromides and bromochalcones with aldoximes. The functionality switching from oxime ethers to phenolic group driven by solvents or temperature was found to be fascinating.

### Contents

1. Introduction to palladium-catalysed C –O cross-coupling reaction 2. Palladium-catalysed rapid methoxylation and trideuteriomethoxylation of bromochalcones: uncovered the catalytic activity of Pd/*t*BuXPhos catalyst system 3. Synthesis of novel chalcones through palladium-catalysed C-O cross-coupling reaction of bromochalcones with ethyl acetohydroxamate 4. Ketoxime: as nucleophilic coupling partner in palladium-catalysed C-O cross-coupling reaction with aryl bromides and bromochalcones 5. Aldoximes: as nucleophilic coupling partner and hydroxide surrogate in palladium-catalysed C –O cross-coupling reaction with aryl bromides and bromochalcones.

30. SACHDEVA (Tanisha)  
**Design, synthesis and characterization of novel phenothiazine derivatives and their potential material and biological applications.**  
 Supervisor: Prof. M. D. Molton  
Th 24392

### Abstract (Not Verified)

The thesis entitled “Design, synthesis and characterization of novel phenothiazine derivatives and their potential material and biological applications” emphasises on the development of novel phenothiazine based derivatives and their applications as potential smart material and biologically active scaffold. Novel push-pull based phenothiazine derivatives were designed and synthesized. Several aryl groups with varied electronic and steric factors were introduced on phenothiazine ring in order to fine tune its donor ability. Suzuki reaction between 7-bromo-10-ethyl-10H-phenothiazine-3-carbaldehyde and different arylboronic acids afforded novel aryl substituted phenothiazine-aldehydes. These newly synthesized phenothiazine aldehydes were utilised for the preparation of various phenothiazine derivatives bearing different acceptor groups including benzothiazolyhydrazones, 2,4-dinitrophenylhydrazones, chalcones and benzothiazoles. These acceptor groups were introduced in order to alter the push-pull behaviour. Phenothiazine pyridylhydrazones were also synthesized which were utilized for the preparation of phenothiazine based triazolopyridine derivatives. All the novel compounds were synthesized in moderate to good yields and were characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, HRMS and IR spectroscopy. Some of these compounds displayed Mega stokes shift which makes them potential candidates for bioimaging applications and fabrication of optoelectronic devices. These derivatives also exhibited moderate to good thermal stability. Some of the derivatives displayed aggregation-induced emission enhancement behaviour. Novel phenothiazine aldehydes were found to be efficient moisture sensing probes for the detection of moisture in common organic solvent. Phenothiazine based pyridylhydrazones and benzothiazole derivatives displayed reversible acidochromism in solution as well as solid state and may have application as acid-base switches. Moreover, D-π-A based phenothiazine derivatives bearing 2-hydrazinobenzothiazole, 2,4-dinitrophenyl and chalcone as acceptor units



displayed multi-stimuli responses indicating their potential as security inks, fluorescent sensors, pressure sensors, data storage and optoelectronic devices. Further, phenothiazine based triazolopyridine derivative with appended phenyl ring on phenothiazine displayed considerable cytotoxic activity and apoptotic induction effects against breast cancer cell line.

### Contents

1. Introduction 2. Design, synthesis and characterization of novel phenothiazine aldehydes and their application as moisture sensing probes 3. Design, synthesis and characterization of novel phenothiazine hydrazones and their applications as potential smart materials 3A. Logic gate based phenothiazine pyridylhydrazones: halochromism in solution and solid state 3B. Multi-stimuli response displaying novel phenothiazine based non-planar D- $\pi$ -A hydrazones: synthesis, characterization, photophysical and thermal studies 4. Design, synthesis and characterization of multistimuli responsive D- $\pi$  phenothiazine chalcone derivatives 5. Design, synthesis and characterization of D-A based novel phenothiazine-benzothiazole derivatives and their application as reversible acid/base sensors 6. Design, synthesis and characterization of novel phenothiazine based triazolopyridine derivatives: evaluation of anti-breast cancer activity on human breast carcinoma 7. Summary and conclusions. .List of publications.

31. SAINI (Kapil Mohan)  
**Novel Strategies for the Regioselective Synthesis of Carbocycles and Heterocycles by Tandem Cyclization.**  
 Supervisor: Prof. Akhilesh Kumar Verma  
Th 24922

### Abstract (Not Verified)

The present thesis entitled “Novel Strategies for the Regioselective Synthesis of Carbocycles and Heterocycles by Tandem Cyclization” describes a novel cascade synthetic methodology for the synthesis of rigid molecular structure. These motifs are critical to advances in the development of broad range of biologically and pharmaceutically important benzothiazolylidene, 1,3-benzothiazines, amino-indinones and quinoxalines analogues. we have established a versatile and environmentally benign tandem protocol which provided a broad range of highly functionalized benzothiazolylidene benzamide derviatives using mild reaction conditions with excellent regioselectivity in good to excellent yields. Further, we have disclosed a mild, organic solvent-free, and base-free, one-pot methodology for the regioselective ring closure of ortho-alkynylanilines with isothiocyanates enabled by the carbon-carbon triple bond activation using iodine. We have designed the base promoted intramolecular ring closure of readily accessible ortho-alkynylaldehyde with a broad range of aromatic and aliphatic amines for the synthesis of substituted amino-1H-indenone with high functional group tolerance and good yield. The (2-alkynyl)-aryldimines gave the regioselective ring closure rather than 6-endo-dig cyclization. Next, we have demonstrated an efficient transition-metal-free one-pot domino approach for the synthesis of diversely substituted furo-fused quinoxalines. The strategy involves the in situ alknlylation followed by 5-endo-dig intramolecular cyclization in the presence of trifluoroacetic acid. we have also achieved the Brønsted-Lowry acid mediated tandem cyclization/C=C bond cleavage of functionalized amino-indenones for the synthesis of pyrrolo[1,2-a]quinoxalines. After successful accomplishment of above goal we have developed one-pot sequential cross-coupling reactions of sterically hindered tetrabromothiophene with boronic

acid and alkyne/alkene using palladium catalyst. Then, we have realized a new regioselectivity of Ag-catalyzed intramolecular tandem electrophilic cycloisomerization of 2,5-diaryl-3,4-bis(arylethynyl) thiophene to form benzoindenothiophene. Benzoindenothiophene was further utilized for the synthesis of bibenzo indeno-thiophenes through C-H activation in the presence of Au(I)-catalyst using a concerted metallation-deprotonation and deprotonation-metallation mechanism.

### Contents

1A. On water: metal-free synthesis of highly functionalized benothiazolidene from ortho-haloanilines 2B. On water: iodine-mediated direct construction of 1,3-benzothiazines from ortho-alkynylanilines by regiodelective 6-exo-dig cyclization 2. Transition-metal-free reverse reactivity of (2-alkynyl)-arylaldehydes: assembly of functionalized amino-indinones, cyclopentaquinolinone and cyclopentapyridinone 3A. TFA-mediated one-pot synthesis of furo-fused quinoxalines/pyrazines 3B. TFA-mediated ring opening reactions of functionalized amino-indinones for the synthesis of 4-substituted methylpyrrolo[1,2-a]quinoxalines 4A. Pd-catalyzed one-pot sequential cross-coupling reactions of tetrabromothiophene 4B. Ag-catalysed tandem electrophilic cycloisomerization and Au-catalysed double C-H activation. Summary of the work

### 32. SATISH CHAND

#### **Synthesis, Spectral Characterization and Molecular Modelling of Cobalt(II), Nickel(II), Copper(II) and Zinc(II) Complexes of Nitrogen, Oxygen and Sulphur Containing Tetradentate Schiff's Base Ligands.**

Supervisor: Prof. Ramesh Chandra and Dr. Sulekh Chandra

Th 24411

#### *Abstract (Not Verified)*

Nitrogen, oxygen and sulphur containing tetradentate Schiff's base ligands L1-L4 were successfully synthesized and characterized by ESI-Mass, <sup>1</sup>H NMR and IR spectra. Their cobalt(II), nickel(II), copper(II) and zinc(II) complexes were synthesized and characterized by elemental analysis, molar conductance, magnetic susceptibility measurements, ESI-Mass, IR, <sup>1</sup>H NMR and EPR spectra. Molar conductances of metal complexes in DMSO indicated their non-electrolytic behaviour. Octahedral geometry was assigned to CO(II) and Ni(II) complexes, tetragonal geometry for Cu(II) complexes and tetrahedral geometry for Zn(II) complexes. TGA curves of the metal complexes of ligands L1-L4 showed better thermal stability than ligands. Geometries of all the ligands L1-L4 and their metal complexes were successfully optimized with respect to energy taking the 6-31+(g,p) basis set in Gaussian 09W programme in gaseous phase. Ligand L1 and its metal complexes were examined against the human pathogenic, Gram negative bacteria i.e. Escherichia coli, Yersinia enterocolitica, Klebsiella pneumoniae and Salmonella typhi and Gram positive bacteria i.e. Listeria monocytogenes and Enterococcus faecalis. The antibacterial screening of the compounds led to the conclusion that Nickel(II) and Copper(II) complexes show comparable activity against L. monocytogenes, E. coli and K. pneumoniae, while cobalt(II) complexes exhibited high activity against Y. enterocolitica and S. typhi, whereas Zinc complex was found active against E. faecalis only. Ligand L2 and its metal complexes were screened against the Gram negative bacteria i.e. Y. enterocolitica, S. typhi, K. pneumoniae and E. coli. The Cobalt(II) complexes were found most active against Y. enterocolitica, K. pneumoniae and E. coli. Against S. typhi, Nickel(II) complex was found the most active one.

Copper(II) and cobalt(II) complexes of ligand L3 were found most active against both the studied Gram positive bacteria i.e. *L. monocytogenes* and *E. faecalis*. BSA binding study of metal complexes of ligand L4 was done.

*Contents*

1. Introduction 2. Synthesis and characterization of ligand L1 3. Experimental 4. Experimental 5. Experimental 6. Experimental 7. Summary and conclusions.

33. SHABIR (Javed)  
**Design and Development of Nanostructured Materials for Catalytic Applications.**  
 Supervisor: Prof. Subho Mazumdar  
Th 24389

*Abstract*  
*(Not Verified)*

The idea of utilizing nanostructured materials has attracted a lot of attention for their application in the field of catalysis. In this thesis, we have developed a variety of nanostructured materials for potential applications in nanocatalysis. Chapter 1 describes the introduction and review of the literature. Chapter 2 is about characterization techniques used. Chapter 3 describes the synthesis of amine functionalized wrinkled silica nanospheres and their application as a solid base catalyst. Chapter 4 is about the synthesis of fibrous cubic silica particles and their applications as a recoverable nanocatalyst. Chapter 5 describes the synthesis of silver nanoparticles using nitrilotriacetic acid in an aqueous medium. Chapter 6 demonstrate the synthesis of graphene coated fibrous silica and its application for the synthesis of 3-amino alkylated indoles. Chapter 7 describes the preparation of well dispersed RuPd alloy nanoparticles stabilized with 2-D reduced graphene oxide and its applications as a recoverable catalyst. Chapter 8 concludes the brief overview of the thesis.

*Contents*

1. Introduction and review of the literature 2. Instrumentation 3. Development of amine functionalized wrinkled silica nanospheres ( $\mu\text{SiO}_2\text{-NH}_2$ ) and their application as an efficient and recyclable solid base catalyst 4. Development of fibrous silica cubes ( $\text{eSiO}_2\text{@KCC-1}$ ) with catalytically efficient silver nanoparticles for multiple reduction and degradation reactions 5. Nitrilotriacetic acid assisted one step synthesis of highly stable silver nanoparticle in an aqueous medium: an investigation of catalytic activity 6. Graphene oxide coated fibrous silica ( $\text{GO@fSiO}_2$ ) anchored with amine terminated ionic liquid: and efficient and recyclable catalyst for the synthesis of 3-amino alkylated indoles via mannich-type reaction 7.  $\text{Ru}_x\text{Pd}_y$  alloy nanoparticles uniformly anchored on graphene nanosheets ( $\text{Ru}_x\text{Pd}_y\text{@G}$ ): an efficient and recyclable catalyst 8. Conclusion and list of publications.

34. SHARMA (Pankaj)  
**Studies on Exploration of Synthetic Strategies for the Development of Some Novel Biologically Interesting Natural, Marine Natural and Herbal Compounds and Synthesis of their Derivatives.**  
 Supervisor: Dr. Sunita Bhagat  
Th 24383

*Abstract*  
(Not Verified)

The thesis entitled “Studies on Exploration of Synthetic Strategies for the Development of Some Novel Biologically Interesting Natural, Marine Natural and Herbal Compounds and Synthesis of their Derivatives” has been divided into five chapters. In chapter 1 we have focused on first total synthesis of methyl (Z)-3-(1-acetyl-9H-pyrido[3,4-b]indole-3-carboxamido) acrylate isolated from *Stellaria dichotoma* var. *lanceolata*. by Shung and co workers. This compound is known to possess anti-inflammatory activity. We have produced an interesting, efficient, simple and widely applicable strategy for its total synthesis and analogues. In Chapter 2 a concise, regioselective and highly efficient strategy for the construction of 6-bromo-5-methoxy-1H-indole-3-carboxylic acid has been developed through trifluoroacetylated indole driven hydrolysis. Bromo indoles bearing carboxylic acid group were further functionalized in amide derivatives by using various aromatic/aliphatic amines through conventional and ultrasonic irradiation. In Chapter 3 we have reported the first total synthesis of 2-amino-3-(4-((6-bromo-5-hydroxy-1H-indole-3-carbonyl) oxy) phenyl) propanoic acid isolated from marine ascidian *Herdmania momus* by Jung and co workers. This compound is known to possess anti-inflammatory activity. We have strategically designed its total synthesis of biological interest. It should be noted that methodology described here can be used for the synthesis of various natural products. Chapter 4 deals with the synthesis of  $\alpha$ -hydroxysuccinamic acid isolated from *E.Jambolana* and its structural analogs for the assessment of their antidiabetic potential in STZ induced diabetic rats. In the present invention we have prepared 4-amino-2-hydroxy-4-oxobutanoic acid, a synthetic alpha hydroxy succinamic acid, the active pharmaceutical ingredient in the management of diabetes mellitus. In Chapter 5 we have summarized an overview on detailed description about recent highlights in electrophilic fluorination with 1-fluoro-2,4,6-trimethylpyridinium tetrafluoroborate and NFSI (N-fluorobenzenesulfonamide) reagents directed towards the synthesis of different heterocycles.

*Contents*

1. First total synthesis of methyl (Z) -3-(1acetyl-9H-pyrido[3,4-b]indole-3-carboxamido) acrylate, a  $\beta$ -carboline alkaloid and its derivatives of biological interest
  2. A concise and regioselective synthesis of 6-bromo-5-methoxy-1H-indole-3-carboxylic acid derivative: strategic development of core moiety of marine natural product
  3. First total synthesis of 2-amino-3-(4-((6-bromo-5-hydroxy-1H-indole-3-carbonyl) oxy) phenyl) propanoic acid, a marine derived natural product
  4. Synthesis of  $\alpha$ -hydroxy structural analogues for the assessment of their anti-diabetic potential in STZ induced diabetic rats
  5. Recent highlights in electrophilic fluorination with 1-fluoro-2,4,6-trimethylpyridinium tetrafluoroborate and NFSI (N-fluorobenzenesulfonimide) reagents directed towards the synthesis of heterocycles; and overview .Summary and list of publications.
35. SHARMA (Shivalika)  
**Multi-Electron Anisotropic Quantum Dots and Hydrogenic Systems in Magnetic Field via Multipole Expansion of Coulomb Interactions Under Full-Scale Fermion Exchange Symmetry.**  
 Supervisor: Dr. Ram Kuntal Hazra  
Th 24395

*Abstract*  
(Not Verified)

This thesis presents a distinct and effective methodology to solve Schrodinger equation of multi-electron 3-D anisotropic quantum dots and Hydrogenic systems exactly in presence of arbitrary magnetic field. Chapter 1 aims to survey holistic background on quantum dots, various approximate methods of many-body theory, symmetry and statistics of quantum particles and mathematical tools. Chapter 2 presents exact formalism of e-e interactions for a 3-D parabolic dot into a terminating finitely summed Lauricella functions in presence of arbitrary magnetic field. Chapter 3 covers the investigation of e-e interaction in various domains of confinement frequency, mass of electron and dielectric constant of 3-D parabolic quantum dots in transverse magnetic field. The level spacing distribution, specific heat and magnetization are also studied. Chapter 4 presents exact formalism for 3-D N-e anisotropic dot by recasting the Hamiltonian in eigen-basis of Whittaker-M function. Coulomb interaction is exploited using multipole expansion into finite single-summed Lauricella function. Chapter 5 deals with the studies of energy spectra and thermodynamic properties of 3-D N-e spherical and axial quantum dots. Chapter 6 encloses investigation of chemical potential and addition energy plots of spherical and ellipsoidal quantum dots (GaAs, atom-like) by varying magnetic field and number of electrons. Chapter 7 encapsulates analytical treatment to 3-D N-e anisotropic dot with full-scale implementation of Pauli exclusion principle in high carrier density. Chapter 8 covers analysis of crucial parameters like fermionic exchange symmetry, geometry of the dot, coulomb interaction, mass of electron, dielectric constant and cyclotron frequency on electronic structure of N-e quantum dots (ZnO, CdSe, atom-like, GaAs). Chapter 9 accounts chemical potential and addition energies of N=1-9 interacting electrons for spherical and ellipsoidal quantum dot for different magnetic field domains. Chapter 10 includes theoretical development of ground state energies of He and its isoelectronic ions upto second order perturbation calculations.

*Contents*

1. Introduction 2. Theoretical development of 3-D 2-e quantum dots 3. Electronic spectra and thermodynamic properties of 3-D 2-e... 4. Theoretical development of 3-D N-e anisotropic quantum dots 5. Electronic spectra and thermodynamic properties 3-D N-e... 6. Chemical potential and shell structure of 3-D N-e anisotropic... 7. Theoretical development of 3-D multi-election (N=1-10)..... 8. Electronic spectra and thermodynamic properties of 3-D multi..... 9. Chemical potential and shell structure of 3-D multi-electron... 10. Ground state energies of helium and iso-electronic ions upto..... Appendix, Bibliography and list of publications.

36. SINGH (Aarushi)  
**Synthesis of Biologically Active Pyrazinoindoles and its Mechanistic Interaction Studies.**  
 Supervisors: Prof. Ramesh Chandra and Dr. Rakeshwar Bandichhor  
Th 24923

*Contents*

1. Introduction 2. Review of and literature 3. Aim and objectives 4. Pharmacological evaluation of novel indoline scaffold based antibacterial compound using chemoinformatics approach and stereoselective N-acbstitued indoles 5. Design and synthesis of stereoselective pyrazinoindoles using HFIP via microwave mediated approach 6. Probing the interaction of biologically active pyrazinoindole derivative

with bovine serum albumin: A biophysical approach Novel pyrazinoindoles derivatives as antibacterial agents: biological evaluation and molecular docking studies .Appendix 3, summary and research publications

37. SINGH (Balram)  
**Synthesis of Carbohydrate-based Cationic Amphiphiles, Styrene C-Glycosides and Study of Antimicrobial & DNA-Binding of Some of Them.**  
 Supervisor: Dr. Indrajit Roy  
Th 24412

*Abstract*  
 (Not Verified)

Cationic amphiphiles bearing cleavable ester linkages between the hydrophilic head group (amino acid) and the hydrocarbon tail (alkyl chain) with carbohydrate spacers that showed good antimicrobial activity against human pathogenic microbes i.e. *L. donovani* causing leishmaniasis and *M. tuberculosis* causing tuberculosis. These novel compounds showed significant anti-leishmanial activity against *L. donovani* promastigotes. Cytotoxicity study reveals that these cationic amphiphiles do not inhibit the growth of human THP1 cell line even at higher concentrations. Cationic amphiphiles bearing cleavable ester linkages between the hydrophilic head group (amino acid) and the hydrocarbon tail (alkyl chain) with carbohydrate spacers. These cationic amphiphiles are highly water soluble and self-aggregates in water to form micelles. The critical aggregation concentration (CAC) values of these surfactants were found to be very low and were many folds smaller than the corresponding analog. These properties make the newly synthesized amphiphiles potentially superior disinfectants and antiseptics for various biomedical and biotechnological applications. The potential optically cleavable amphiphilic system was synthesized. These amphiphilic systems are water soluble and self-assemble in aqueous buffer forming micellar aggregates bearing a net positive charge. The amphiphiles employ naturally occurring and non-toxic amino acid as a surface group; glucose and the photolabile o-NB group as a spacer; and long alkyl chain as the hydrophobic tail. These systems can achieve reversible DNA binding by using photolabile multivalent groups, which release DNA by degrading and charge-reversing multivalency. In addition to this, these systems can also dissolve non-polar therapeutic drugs in aqueous solution in their core through complementary electrostatic interactions and they can also release their target very rapidly upon long-wavelength UV irradiation ( $\lambda = 350$  nm). A simple, efficient and eco-friendly route for the exclusive synthesis of (*E*)-1-phenyl-2-( $\beta$ -D-glucopyranosyl)ethenes from native sugars in excellent to good overall yields using Bamford-Stevens reaction in one of the crucial steps.

*Contents*

1. Antitubercular and antileishmanial activities of micelles of peptide-sugar based cationic amphiphiles 2. DNA binding study on micellar aggregates of uracil based glucopyranose glycinates & lysinates 3. Potential optically triggerable carbohydrate based micellar aggregate 4. Grenner synthesis of (*E*)-1-phenyl-2-( $\beta$ -D-glucopyranosyl)ethane . List of publications

38. SOOD (Damini)  
**Development of an Anti-Cancer Drug Noscapine: Biophysical and In Silico Studies.**  
 Supervisor: Dr. Sujata K. Dass  
Th 24409

*Abstract*  
(Not Verified)

Cancer is the untamable growth of abnormal cells and consequent deprivation of nutrients for the normal cells. Noscapine has been known to inhibit the tumor progression by interacting with the microtubules during mitosis. The recent developments have led us to carry out research to decipher the binding properties of Noscapine and its analogues with various model protein as well as DNA to uncover its unknown mechanisms of interaction and overcome its limitations. The synthesis of Noscapine loaded biodegradable nanoparticles will be successful in dealing with lowering the dosage and offer a targeted delivery of Noscapine. These results culminate into a successful model in developing Noscapine as an anti-cancer drug by offering new insights and solutions to its previously known limitations. The multi-spectroscopic studies demonstrated that Noscapine and its analogues show moderate binding (order of  $10^3 \text{ M}^{-1}$ ) with model proteins (BSA and Lysozyme). Noscapine binds to DNA via intercalation in vitro without majorly affecting the DNA stability. Moreover, molecular modelling studies showed potential binding of the Noscapine with BSA and lysozyme. In addition, molecular dynamic simulation validated the stability of the complex. This is essential for the drug transportation and for the drug to exert its therapeutic effect. The chitosan coated magnetic nanoparticles showed high loading capacity with sustained drug release. Overall compiling these studies elucidates the mechanism of interaction and drug delivery application of noscapine and its potential derivatives with different human proteins; study required to move a step closer in the clinical study of Noscapine and establishing it as a successful anti-cancer drug.

*Contents*

1. Introduction 2. Interaction study of bromo-noscapine with bovine serum albumin employing spectroscopic and chemoinformatics approaches 3. Deciphering the binding mechanism of lysozyme with noscapine: spectroscopic and chemoinformatics approaches 4. Synthesis, characterization and anti-oxidant activity of chitosan coated magnetic nanoparticles for the targeted drug delivery of noscapine 5. The mechanistic study of noscapine-CT DNA complex using multi-spectroscopic methods and molecular docking analysis. .Summary and research publications.

39. TYAGI (Monika)  
**Synthesis, Characterisation and Biological Screening of Transition Metal Complexes with Schiff's base ligands.**  
 Supervisors: Prof. Ramesh Chandra and Dr. Sulekh Chandra  
Th 24390

*Abstract*  
(Not Verified)

Mn(II), Co(II), Ni(II) and Cu(II) complexes with Schiff's base ligands (L1-L5), have been synthesised. Complexes were characterized by elemental analysis, molar conductance measurements, mass, ir, epr and electronic spectral studies. The geometry of complexes has been optimised by using Gaussian 09 W. Carbon, hydrogen and nitrogen was analysed by CHN analyser. The ELICO (type CM82T) conductivity bridge was used for measuring molar conductances. IR spectra were recorded in range of  $4000\text{-}400 \text{ cm}^{-1}$  on the IR instrument in KBr pellets. DMSO as solvent was used for recording electronic spectra. LC-ESI-MS based analysis was done for calculating electronic impact mass spectrum at JNU. EPR spectrum of metal complexes as polycrystalline samples was recorded by using DPPH as g

marker in IIT Bombay. Ligand L1, 3-(Benzo[b]thiophen-2-yliminomethyl)-benzene-1,2-diol was synthesised by condensation reaction in between methanolic solution of 2,3-dihydroxybenzaldehyde and aminobenzothiazole. Ligand L2, 3-[Mercapto-[1,3,4]thiadiazol-2-ylimino)-methyl]-benzene-1,2-diol was synthesised by condensation reaction in between methanolic solution of 2,3-dihydroxybenzaldehyde and 5-amino-1,3,4-thiadiazole-2-thiol. Ligand L3, 3-[(4H-[1,2,4]Triazol-3-ylimino)-methyl]-benzene-1,2-diol was synthesised by condensation reaction in between methanolic solution of 2,3-dihydroxybenzaldehyde and 4-H-1,2,4-Triazol-3-amine. Ligand L4, 2-(1-Phenyl-pyridin-2-yl-methylene)-amino]-[1,3,4]thiadiazole-2-thiol, was synthesised by condensation reaction in between methanolic solution of 2-benzoyl pyridine and the hot methanolic solution of 5-amino-1,3,4-thiadiazole-2-thiol. Ligand L5, 5-[(1H-Indol-3-ylmethylene)-amino]-[1,3,4]thiadiazole-2-thiol was synthesised by condensation reaction in between methanolic solution of Indole-3-carbaldehyde and 5-amino-1,3,4-thiadiazole-2-thiol. The novel research work is the screening of all the synthesised ligands and their Mn(II), Co(II), Ni(II) and Cu(II) complexes against fungal species i.e. *Aspergillus niger* and *Candida tropicalis* by using of "Food poison method" and bacterial species i.e. *P. aeruginosa*, *S. pyogenes* and *B. subtilis* by using "well diffusion method". The activity was checked by measuring growth inhibition zone. Antimicrobial screening data indicates the antimicrobial properties of both the ligand as well as Metal complexes. Metal complexes was found more potent against bacteria and fungi as compare to the parent ligand.

#### Contents

1. An introductory overview on Schiff's base ligands 2. Synthesis of schiff's base ligands (L<sup>1</sup>-L<sup>5</sup>) and their characterisation 3. Mn(II) complexes:- synthesis with schiff's base ligands (L<sup>1</sup>-L<sup>5</sup>) and their characterisation 4. Co(II) complexes: synthesis with Schiff's base ligands (L<sup>1</sup>-L<sup>5</sup>) and their characterisation 5. Ni (II) complexes:- synthesis with schiff's base ligands (L<sup>1</sup>-L<sup>5</sup>) and their characterisation 6. CU(II) complexes:- synthesis with schiff's base ligands (L<sup>1</sup>-L<sup>5</sup>) and their characterisation 7. Microbiological screening:-antifungal and antibacterial activity.

40.

VIJAY KUMAR

#### **Development of Chemosensors Bearing Different Fluorophores for the Selective Detection of Assorted Analytes.**

Supervisors: Prof. Rajeev Gupta

Th 24387

#### *Abstract* (Not Verified)

Chapter 1 which provides a brief background of assorted fluorescent chemosensors, available in the literature, for the detection of various cations, anions, explosives and drugs. Chapter 2 describes pyridine-2,6-dicarboxamide based novel fluorescent probes displaying selective binding of Pd<sup>2+</sup> ion in aqueous medium. Collective studies comprising of Job's plots, Benesi-Hildebrand fittings, Stern-Volmer plots and detection limits asserted selective recognition of the Pd(II) ion. These probes further demonstrated potential applications. Chapter 3 presents the synthesis of Pd(II) complexes of pyridine-2,6-dicarboxamide based ligands. These Pd(II) complexes have been used for the selective detection of warfarin (WR), a commercial anticoagulant drug. This work illustrates the application of Pd(II) complexes not only in the excellent sensing of warfarin in organic but also in aqueous medium. Chapter 4 deals with the synthesis of several pyridine-2,6-dicarboxamide based chemosensors. Such receptors acted as the chemosensors for the selective detection



of  $S^{2-}$  ion as well as gaseous  $H_2S$  in primarily aqueous medium. A chemosensor containing appended benzothiazole rings was found highly selective for the detection of  $S^{2-}$  ion as well as gaseous  $H_2S$ . We also illustrate detection of sulfide ion as well as gaseous  $H_2S$  in live cells and paper-strip based sensing. Chapter 5 presents the synthesis of two pyrrole-2-carboxamide based chemosensors. These chemosensors were used for the individual detection of  $Cu^{2+}$ ,  $Al^{3+}$ ,  $Cd^{2+}$  and  $S^{2-}$  ions. Simple synthesis, multi-stimuli response, fast response, solution visualization, and practical detection methods suggested excellent sensing potentials of both the chemosensors. Chapter 6 presented the synthesis of hydroxyl-group-based chemosensors. These chemosensors selective detection of  $Al^{3+}$  and  $Ga^{3+}$  ions. Changes in the absorption and emission spectra of chemosensors in ethanol were easily observable upon the addition of  $Al^{3+}$  and  $Ga^{3+}$  ions. The multi-ionic response and optical visualization of the present chemosensors made them ideal for the practical applications for real samples.

### *Contents*

1. Introduction to chelate-based chemosensors for the selective detection of cations, drugs and assorted analytes 2. Selective fluorescent turn-off sensing of  $Pd^{2+}$  ion by a series of pyridine-2,6-dicarboxamide based tridentate ligands 3. Detection of anticoagulant drug warfarin by palladium complexes of pyridine-2,6-dicarboxamide based ligands 4. Detection of sulphide ion and gaseous  $H_2S$  using a series of pyridine-2,6-dicarboxamide based ligands 5. Fluorescent detection of multiple ions by two related chemosensors: structural elucidations and logic gate applications 6. Turn-on fluorescent sensors for the selective detection of  $Al^{3+}/Ga^{3+}$  and  $PPi$  ions by a series of O-donor ligands. List of publications.