

CHAPTER 55

TECHNOLOGY
APPLIED SCIENCES AND HUMANITIES

Doctoral Theses

01. AGGARWAL (Deepika)
On Convergence Estimates by Some Integral Type Operators.
Supervisor : Prof. Vijay Gupta
Th 25450

Abstract
(Not Verified)

The present thesis deals with the convergence estimates for certain summation Chapter 1 consists the Historical Background of linear positive operators, which are relevant to our further investigations. Chapter-wise summary of the thesis are provided here for groundwork. establish a Voronovskaya type theorem, uniform convergence estimate and also an asymptotic formula. We present here comparative study through graphical representation. of Post-Widder operators, which preserve the test function. Certain well known direct results in terms of modulus of continuity viz. usual, In chapter 4, we establish the quantitative estimates in terms of weighted modulus of continuity, for differences of Baskakov operators with its variants. Also, estimates for mutual differences of these operators are obtained here. Chapter 5 deals with the genuine Lupa,s-Beta operators of integral type. With the help of these operators,one may get different special cases, for different values of γ . Quantitative asymptotic formula, direct estimate in terms of second order modulus of continuity and rate of convergence for functions having derivatives of B'ezier variant are established here. Chapter 6 deals with the (p, q) analogue of the Baskakov-Sz'asz operators and present direct estimate in terms of second order modulus of continuity and also estimate results in weighted spaces.

Contents

1. Introduction 2. Hybrid operators preserving exponential functions 3. Post wider operators preserving the test functions er 4. Difference estimates of baskakov type operators in weighted norm 5. Convergence estimates of certain Lupas-Beta operators 6. Direct estimates for (p,q) - variant of certain hybrid operators. Future work plan. References.

02. BHARDWAJ (Rekha)
Study and Growth of Nano/Micro Structure of Nickel Sulphide Using Hydrothermal Method for Solar Energy Devices.
Supervisor : Prof. Ranjana Jha
Th 25446

Contents

1. Introduction 2. Synthesis and characterization techniques 3. Comparative study of the electrochemical properties of mesoporous 1\D and 3-D Nano structured rhombohedral nickel sulphide in alkaline electrolytes 4. Enhanced electrocatalytic activity of the solvothermally synthesized mesoporous rhombohedral nickel sulphide 5. Hydrothermally prepared nickel disulphide nanoparticles with enhanced areal capacitance 6. Improved electro catalytic performance with enlarged surface area and reduced band gap of caterpillar and cabbage like nickel sulphide nanostructures 7. Trisodium citrate assisted morphology controlled synthesis of nickel sulphide nanoparticles with enhanced cyclic stability as carbonaceous free electrode material 8. Conclusion and future perspective. List of publications

03. BHUSHAN (Medha)

Synthesis and Characterization of Solar Energy Nano Materials.

Supervisor : Prof. Ranjana Jha

Th 25445

Abstract (Not Verified)

The thesis entitled "SYNTHESIS AND CHARACTERIZATION OF SOLAR ENERGY NANO MATERIALS" mainly focuses on the synthesis of different ZnS nanostructures and its characterizations with the aim of applications in solar energy conversion, energy storage devices and photo catalytic degradation. ZnS is a direct band semiconductor. It has amazing chemical stability against hydrolysis and oxidation. ZnS are interesting entities for catalytic applications because all its characteristics are maintained when converted to nano range where they are exposed to fierce environment. Furthermore, ZnS is non toxic and exists in abundance in nature. So, ZnS can be utilised as an imperative catalyst for protection of environment. For any material to be used for energy device applications it has been seen that material used should be at nanoscale, better photocatalyst, and better electrocatalysts. Energy and ecological issues increase high demands on the growth of a sustainable energy system, and better photocatalysts and electrocatalysts are one of the most important ways to realize this goal. This work highlights the engineering of electronic energy state and surface area in the nanoscale regime of ZnS materials, which make them suitable for energy applications. As the performance of electrochemical energy device such as supercapacitors and photocatalytic activities depend strongly on the properties of materials. This study delineates the various parameters like morphology, energy bandgap, charge transfer resistance, different defect states, diffusion coefficient, functional groups adsorbed on the surface of material etc. to assess the performance of supercapacitor electrode and photocatalytic degradation efficiency of ZnS nanostructures. Though, rapid rate of recombination of photogenerated electrons and holes and narrow range of absorption of ZnS nanostructures limit their useful applications as catalysts. To overcome these limitations, ZnS catalysts have been tailored chemically by combining Graphene into ZnS nanoparticles. Graphene hugely affect the structural, surface, optical, electrochemical properties of ZnS nanoparticles.

Contents

1. Introduction 2. Methods and characterization techniques 3. Reduced band gap diffusion controlled spherical n-type ZnS nanoparticles for absorption of UV-Vis region of solar spectrum 4. Ethylenediamine assisted growth of multi dimensional ZnS nanostructure and study of its charge transfer mechanism on supercapacitor electrode and photocatalytic performance 5. Surface activity correlations of mesoporous 3-D hierarchical ZnS nanostructures for enhanced photo and electro catalytic performance 6. Effect of sulphur concentration on structural optical and electrocatalytic properties of ZnS nanoparticles synthesised via thermal decomposition route 7. Graphene doped ZnS nanoparticles with enhanced interfacial charge properties synthesised via simple hydrothermal route for energy applicators 8. Conclusion and future prospects. List of publications.

04. CHAUDHARY (Prachi)
Study of Structural Dielectric and Magneto Electric Properties of Bismuth Ferrite Barium Titanate Cobalt Ferrite Based Materials.
 Supervisor : Prof. O.P. Thakur
Th 25452

Abstract (Not Verified)

The field of research discussed in the present thesis has a tortuous taxonomy and typically involves terms, such as 'multiferroic' and 'magneto-electric'. The current work focuses on the synthesis techniques and the study of structural, dielectric and magneto-electric properties of Bismuth Ferrite, BiFeO₃, Barium Titanate, BaTiO₃, Strontium Bismuth Niobate, SrBi₂Nb₂O₉ and Cobalt Ferrite, CoFe₂O₄ materials to produce new varieties of multi-functional devices, due to their size-dependent chemical and physical properties, which have motivated a whole lot of current researchers to work in the area of magneto-electric multiferroics. Multiferroics are the materials having at-least two ferroic ordering such as ferroelectricity, ferromagnetism and ferroelasticity in the same phase. BiFeO₃ is a most promising multiferroic material. However, it suffers from a few limitations such as poor perovskite phase stability, weak magneto-electric coupling and low electrical resistivity. To overcome these drawbacks, we have synthesized and studied the following systems: solid solution BiFeO₃-BaTiO₃, ternary systems BiFeO₃-BaTiO₃/CoFe₂O₄ and Nb₂O₅ modified BiFeO₃-BaTiO₃ system. Multiferroic materials might show a coupling effect contributing to potential implementations in ferroelectric and magnetic devices namely resonators, transducers, information storage, electromagnetic interference filter, field sensors, and spintronics. In particular, the current interest lies in the existence of cross-coupling between the magnetic and electrical order parameters leading to a unique magneto-electric effect in the material. Improving its magnetic features without affecting the ferroelectric behaviour is essential for use in real-life device applications. Properties of materials are found to largely depend upon particle size, shape, phase purity and crystal symmetry, so more focus should be laid on the synthesis of pure phase homogeneous shape and size. In the wide field of multiferroics, the appropriate substitution of corresponding ions will enhance its ferroelectric and magnetic features. Further improvement in the ferroelectric and

magnetic properties may be helpful for enhanced performance of devices such as NVRAM.

Contents

1. Introduction and motivation 2. Experimental: synthesis and characterization details 3. Structural, dielectric, energy storage and magneto-electric coupling analysis in $(\text{BiFO}_3\text{-BaTiO}_3)/\text{CoFe}_2\text{O}_4$ composites 4. A study on structural microstructural and multiferroic properties of $\text{SrBi}_2\text{Nb}_2\text{O}_9\text{-CoFe}_2\text{O}_4$ composites 5. Structural microstructural dielectric magnetic and electrical properties of NB_2O_5 - modified $\text{BiFeO}_3\text{-BaTiO}_3$ solid 6. Summary and future scope of work. List of publications. Copies of reprints of published research papers included in thesis.

05. CHUGH (Bhawna)

Study of Mechanism of Corrosion Inhibition of Some Hetero Atom Containing Compounds.

Supervisors : Prof. Sanjeev Thakur and Dr. Ashish Kumar Singh

Th 25444

Abstract (Not Verified)

The thesis entitled “Study of mechanism of corrosion inhibition of some Hetero-atom containing compounds” deals with the study of various efficient corrosion inhibitors and their anticorrosion performance on mild steel (MS) in 1M HCl/0.5 M H₂SO₄ solution by employing different techniques. Corrosion is a natural process that leads to the deterioration of substances by means of chemical modifications by the environment. The imprints of corrosion are diverse which causes structural collapse or breakdown of bridges, cars, aircraft, etc. MS is very useful in industrial implications because of its exquisite mechanical properties, easy availability, and cost-effectiveness. But, despite its wide application, it is easily affected in acid solutions which are frequently employed for many industrial processes like pickling, cleaning, and descaling. Thus, there is a huge demand for discovering certain strategies for combating the corrosion of MS in acidic medium. A number of organic inhibitors have been proclaimed as competent corrosion inhibitors for MS in acidic environments. The majority of commonly used inhibitors are organic molecules comprising pi bonds, aromatic groups, and heteroatoms, for example, O, N, or S, which promotes the adsorption over the metal surface. The research work embodied in the present thesis focusses on the investigation of some Benzothiazole derivatives, Bis-thiadiazole derivatives, and Pyrazine carbohydrazones as inhibitors for MS in 1M HCl and Cinnamaldehyde modified chitosans in 0.5 M H₂SO₄. Various techniques such as weight loss, Potentiodynamic Polarization, and Electrochemical Impedance Spectroscopy have been employed to estimate the anticorrosion performance of synthesized inhibitors. Surface characterization such as Scanning electron microscopy with energy dispersive spectroscopy (SEM-EDX), and X-ray photoelectron spectroscopy (XPS) reflected the protective barrier of inhibitors on the MS

surface mitigating corrosion. The theoretical findings such as density functional theory (DFT), Fukui indices, and molecular dynamics (MD) have been described to provide good agreement with different experimental techniques.

Contents

1. Introduction 2. Experimental 3. An exploration about interaction of mild steel with hydrochloric acid in presence of N-(BENZO [d] thiophene -2-YL)-1 phenylethan-1- imines 4. Comparative investigation of corrosion-mitigating behaviour of thiadiazole derived BIS-SCHIFF based for mild steel in acid medium: experimental, theoretical and surface study 5. Comprehensive study about anti corrosion behaviour of pyrazine carbohydrazide: gravimetric electrochemical surface and theoretical study 6. Relation of degree of substitution and metal protecting ability of cinnamaldehyde modified chitosan 7. Summary and scope of future work. List of publications.

06. DABAS (Samiksha)
Investigations of Structural Dielectric and Magnetoelctirc Properties of Multiferroic Bismuth Ferrite Based Materials.
 Supervisor : Prof. O.P. Thakur
Th 25453

Abstract *(Not Verified)*

The present study deals with a comprehensive analysis of the lead free and doped BFO based composite system and solid solutions. Here, focus of the present research is on quantification of ME coupling coefficient and optimization of useful energy storage density which is of immense importance in future device applications. The inter-conversion of Fe ions amongst themselves require charge compensation and thereupon create oxygen vacancies. This hinders the use of single phase multiferroic Bismuth Ferrite (BFO) for the potential application purposes. The Bi-site doping of rare earths can effectively destroy or subdue the cycloidal spin structure and consequently releases weak ferromagnetism in the crystal lattice. Further, higher valence ion doping at the Fe-site curtails oxygen vacancies and suppresses the cycloidal spin leading to improved magnetic response. Subsequently, the potential established methods for BF to strengthen its ferroelectric and magnetic properties include doping (Bi-, Fe- and both Bi- & Fe- sites), solid solutions including binary and ternary systems and composites formation. Thus, the choice of materials aims at reducing the inherent limitations of bulk BFO such as enhancing magnetic response of the G-type antiferromagnetic bulk BFO, reducing limitations arising due to high leakage current, improving the overall multiferroic properties by the suitable doping or composite formation. Further, solid state reaction approach is utilized to synthesize compositions namely, (a) BiFeO₃-CoFe₂O₄ (b) Mn-doped BiFeO₃ and Mn-doped BiFeO₃-BaTiO₃ solid solutions, (c) Gd-doped BiFeO₃-BaTiO₃ solid solutions. The material characteristics are corroborated with an in-depth analysis of structural properties, ferroelectric loop and the calculation of energy storage density, magnetic properties, ME coupling coefficient, dielectric properties, and impedance studies.

Contents

1. Introduction and research objectives 2. Experimental details: materials synthesis and characterization 3. Structure magnetic and dielectric properties of $\text{BiFeO}_3\text{-CoFe}_2\text{O}_4$ composites 4. Effect of Mn-dopping on the structural magnetic dielectric properties magnetoelectric coupling coefficient and energy storage analysis in BiFeO_3 and $\text{BiFeO}_3\text{-BaTiO}_3$ 5. Structural, magnetic, dielectric properties, impedance spectroscopy and conductivity analysis in GD-doped $\text{BiFeO}_3\text{-BaTiO}_3$ 6. Structure and future scope of work. List of research publications. Copies of reprints of published research papers included in thesis.

07. DAYANAND

Synthesis and Characterization of Iron Oxide and Iron Oxide Carbon Nano Composites by Spray Pyrolysis.

Superviso : Prof. O.P. Thakur

Th 25447

Abstract

(Verified)

In recent years, iron oxide (Fe_2O_3) has attracted much attention as its different structural and morphological forms have found several technological applications such as ultrahigh magnetic storage devices, magneto-optic sensors gas and humidity sensors, field emission devices etc. Iron oxide exists in different structural forms viz- rhombohedral $\alpha\text{-Fe}_2\text{O}_3$, cubic $\alpha\text{-Fe}_2\text{O}_3$ and Fe_3O_4 etc. Since, the morphology and microstructures are critical factors to bring novel and unique size and shape dependent functional properties, significant attention has been paid for controlled synthesis of nano-materials employing different techniques using variety of pre-cursors. Spray pyrolysis is a widely used technique for producing micro- and nano-scale materials of various kinds such as metals, metal oxides, semi-conductors etc. Because of its a convenient process characteristics compared to other methods like physical and chemical vapour deposition, plasma assisted vapor deposition, laser ablation etc., spray pyrolysis has found tremendous attention in recent times. This technique has an additional advantage that it is possible to obtain particles of varying size distributions and also thin film coatings over large area substrates. In this process, simple pre-cursors could be used to obtain fine particles or uniform coatings over large area in a single step avoiding complicated processes and complex chemical reagents. In the present work, thin films of uniformly distributed Fe_2O_3 nanoparticles have been prepared on single crystal silicon and glass substrates by a spray pyrolysis technique in a single step using a mixture of water and ferrocene dissolved in xylene. The size distribution of nanoparticles is found to be in the range of 20 nm to 30 nm. The crystallinity and band gap of the thin films were investigated using X-ray diffraction, Scanning Electron Microscopy, UV-Visible absorption and Raman spectroscopy techniques. Raman spectroscopy measurements were carried out by two different advanced techniques including Raman area mapping and Raman thermal imaging techniques.

Contents

1. Introduction 2. Spray pyrolysis 3. Characterization techniques 4. Deposition of single phase polycrystalline α -Fe₂O₃ thin films on silicon and silica substrates by spray pyrolysis 5. Raman area and thermal mapping faceted nano crystalline α -Fe₂O₃ thin films deposited by spray pyrolysis 6. Summary and conclusions.

08. MITTAL (Sheena)

Interaction and Propagation of Waves in Compressible Fluids.

Supervisor : Prof. Jasobanta Jena

Th 25449

Abstract (Not Verified)

This thesis consists of five chapters out of which the first chapter is the introductory and contains the overview of the works presented in the thesis. The second chapter is concerned about the interaction of singular surface with characteristic shock in a dusty relaxing gas. Using the singular surface approach, the transport equation for the jump in the first order derivative of the velocity, which is of a Bernoulli type equation is obtained. The solution of the transport equation is discussed considering a particular case. The interaction of the singular surface with the characteristic shock is discussed. The results obtained are analyzed for various dust parameters along with the relaxation effects involved in the flow by performing numerical calculations and depicting the same. The third chapter is related to the application of the simple wave theory to study the shock formation in the small amplitude limit in a non-ideal relaxing gas. For the purpose the first and second order approximations of the flow variables have been evaluated and examined. The fourth chapter is concerned about the interaction of the singular surface with a strong shock in self-gravitating interstellar gas cloud with spherical symmetry. The method of Lie group of transformations is employed to evaluate the forms of the flow variables and the cooling-heating function for an infinitely strong shock. The fifth chapter is concerned about obtaining the self similar solutions using the infinitesimal transformations in the generalized Chaplygin gas, which entails negative pressure and the positive speed of sound. The evolution of acceleration wave in the medium, which is described by the Bernoulli type equation, is derived. The solutions of the equation, which provide insights to the formation of compression waves and expansion waves, are discussed.

Contents

1. Introduction 2. Interaction of a singular with characteristic shock in a relaxing gas with dust particles 3. Rapid pulses through a non ideal relaxing gas 4. Interaction of a singular surface with a strong shock in interstellar gas clouds 5. Evolution of acceleration waves in generalized chaplygin gas. Bibliography.

09. RADHA

Entophytic Actinomycetes Derived Compounds as Potential Therapeutic Agent.

Supervisor : Prof. Ashok K. Dubey

Th 25448

Abstract
(Verified)

Presumably all the plants are associated with microbial communities present within their tissues. Actinobacteria are among the prominent members of the endophytic community of microorganisms. They have been known as potential producer of metabolites with antimicrobial, antioxidant, antimalaria and several other properties. The immense diversity of flora spread over uniquely distinct ecological niches offer an opportunity to access yet unexplored and novel population of actinobacteria for mining of new compounds for therapeutic applications. In this study endophytic actinobacteria have been isolated from the plants that has not been previously explored. The most potent isolate ADR1 was selected and characterised for its ability to produce therapeutically significant metabolites. Isolate ADR1 was identified as *Streptomyces californicus* based upon 16S rRNA sequence which is a new endophytic actinobacterial strain not yet reported from any plant. The metabolites produced by ADR1 showed presence of flavonoids, terpenes, terpenoids, phenols, anthraquinone, anthocyanins, glycosides and alkaloids which are established classes of therapeutically significant compounds. The ADR1 metabolite extract inhibited growth of *Staphylococcus* spp. and *Enterococcus* spp. with MIC₉₀ values in the range of 0.23 ± 0.01 to 5.68 ± 0.20 µg/ml. It also showed inhibition biofilm formation and depletion of preformed biofilm. The metabolite extract possessed antioxidant potential as it scavenged several free radicals. Two novel compounds ADR1-01 and ADR1-02 were isolated from the extract by column chromatography. Spectroscopic analysis of the compounds was carried out using LCMS, FTIR and NMR for structure elucidation. Both the compounds displayed antibacterial, anti-biofilm, antioxidant and antimalaria activity. No haemolysis was observed on sheep blood agar plate. Cytotoxicity of the molecules was estimated against HUH cell line and found to be safe at subinhibitory concentrations. On the basis of theoretical studies done on ADME swiss and TEST online tools both the molecules were found to possess drug likeness properties.

Contents

1. Introduction 2. Review of literature 3. Material and methods 4. Result and discussion 5. Summary 6. Bibliography. Appendices.

10. SHARMA (Deeksha)
Synthesis and Characterization of Anti DevR- Compounds and Their Application in Mycobacterium Tuberculosis.
 Supervisors : Prof. Anjana Sarkar and Dr. Rajesh Kumar Gupta
Th 25443

Abstract
(Verified)

From the beginning of life to present scenario, tuberculosis considered as the world wide disease without any limitation because the treatment is low due

to the heavy thickness of lipid mycobacterial wall & hence the administration of drug inside the mycobacterial cell is challenging. In the present study we focused on the functional and structural role of DevR and Strategy adopted for designing and optimization of anti DevR compounds. The synthesis of 5-amino uracil Schiff's base (11 derivatives) and substituted benzoic thiazolidin-4-one (33 derivatives) with substituted benzaldehyde were purified and characterized by the spectroscopic techniques. Spectral data (IR peaks, ^1H and ^{13}C & Mass) of compounds, their % yield, Melting points were reported. All the synthesized compounds were evaluated for their inhibition viability against aerobic and anaerobic condition using Resazurin Microplate Assay and Hypoxic Resazurin Reduction Assay respectively in *Mycobacterium bovis* strain. Toxicity of compounds is tested in HepG2 cell lines using MTT assay. Only 1-2% toxicity was reported in tested compounds. These results encourage us to carrying forward the testing of these molecules for further study in infection model. The antioxidant study of synthesized compounds by 2, 2-Diphenyl-1-picrylhydrazyl (DPPH) and Phosphomolybdenum assay confirms that tested compounds have capacity to reduce ROS. The testing of synthesized compounds for DevR specificity in DevR over expression conditions in *M.tb*. A novel reporter assay was developed for screening compounds that specifically target DevR activity and not sensor kinase function in *M.tb*. It was found that the four novel compounds designated as A11, are identified to be having potent and specific anti-DevR activity, Notably, many other compounds such as (D3, D4, P3, N8, and N10) are good DevR inhibitors at 96 hours, and studies are needed to convert these potential hit compound to lead compound.

Contents

1. Introduction and literature survey 2. Designing and optimization of Anti-DevR compounds 3. Synthesis and characterization of Anti-DevR compounds 4. Assessment of compound activity on aerobic on aerobic and hypoxia adapted *mycobacterium bovis* BCG 5. Toxicity 6. Antioxidant study of synthesized compounds 7. Target specificity of compounds 8. Conclusion. List of publications.

11. SHASHANK SHEKHAR

Design, Spectral Characterization, DFT and Biological Studies of Transition Metal Complexes of Schiff Bass.

Supervisor : Prof. Anjana Sarkar

Th 25451

Abstract (Verified)

The proliferation in cancer and multidrug-resistant infections amidst personage with the evolution of civilization is an alarming bone of contention. Cancer has long been the pre-eminent core of death worldwide, additionally, it paves the way for a large portion of the microbial infections hence increasing the implications. Nonetheless, the wide rate of multidrug opposition in both diseases entails the development of potential molecules

with intended characteristics that could dodge multidrug-resistant issues. A fruitful methodology in anticancer chemotherapy has been the utilization of drugs with metal as active ingredients that can be utilized to treat multi-resistant infections more effectively. Schiff bases have been the subject of extensive enthusiasm, inferable from their adaptable metal chelating properties, innate organic exercises, and adaptability to alter the structure to tweak it for specific natural applications. With the advent of the modern pharmaceutical industry, biochemical approaches to forestalling and treating disease have procured a new level of prominence in the evolving relationship between microbes and their human hosts. This review gives an insight into some indispensable biological aspects of Schiff bases in light of their antibacterial and anticancer activity and discusses the potential and eventual fate of this class of metallodrugs either as anticancer or antimicrobial specialists. This thesis focuses on the designing, synthesis, and characterization of several ligands and their Schiff base metal complexes. These metal complexes of all Schiff base ligands were also synthesized and characterized by using spectroscopic techniques and molecular modeling. All synthesized ligands and their metal complexes were explored for their antimicrobial activity (antifungal and antibacterial).

Contents

1. Introduction and literature survey 2. Experimental techniques 3. Synthesis and characterization of Schiff base ligands 4. Synthesis spectral characterization and computational studies of Cu(II), Ni(II), and Mn(II) complexes of HLI Schiff base ligand 5. Synthesis spectral characterization and computational studies of Cu(II), Ni(II), Co(II), Mn(II) complexes of HL2 schiff base ligand 6. Synthesis spectral characterization and computational studies of Cu(II), Ni(II), Co(II), Mn(II) complexes of HL3 schiff base ligand 7. Synthesis, spectral characterization and computational studies of Cu(II), Ni(II), Co(II) and Mn(II) complex of HL4 schiff base ligand 8. Conclusion and future scope. List of publications.