

CHAPTER 52
TECHNOLOGY
APPLIED SCIENCES AND HUMANITIES

Doctoral Theses

01. BHASHA
Studies on Preparation and Characterization of Polymer Nanocomposites Functionalized with Graphene.
Supervisors : Dr. Purnima Jain
Th 24177

*Abstract
(Verified)*

Polymer nanocomposites have created quest among researchers over the past few decades due to their exceptional mechanical, thermal, electrical properties and ease of fabrication. Innovation in the field of polymer nanocomposite leads to diverse applications in drug delivery, biosensors, bone regeneration, solar cells, super capacitors etc. A step towards sustainable development; biomimetic approach has been taken into consideration in which vital role is played by the integration of nan fillers in biopolymers. The evolution of eco-friendly and cost-efficient energy storage devices is eminent because of depletion of ozone layer and environmental issues. Biopolymer nanocomposites are the most auspicious aspirant to intercept hazardous situations which undergo a revolutionary shift to evolve sustainable materials. In the present scenario the utilization of biopolymers are facilitated by the functionalization of nano-filler by different types of methods which can eradicate agglomeration and enhance thermal, mechanical and electrical properties. Biopolymer nanocomposites have been used as an alternative over conventional polymers due to their environmental friendly, biocompatibility and non-toxic characteristics. The inclusion of nano filler like silicates, carbon nanotubes (CNTs), metal oxide nanoparticles and graphene based nano platelets can readily enhance the physical, thermal, mechanical and electrical properties of biopolymers. The current research work unveils the concoction of biopolymer nanocomposites reinforced with graphene and its derivatives, and also to investigate the thermal, mechanical, morphological and rheological properties. Poly (Vinyl Alcohol) (PVA) has been used as a biopolymer matrix and graphene is used as reinforcing nanofiller. PVA nanocomposites result in impervious enhancement in mechanical properties such as tensile strength, young's modulus and thermal resistance. The outstanding properties of PVA nanocomposites are attributed to the incorporation of graphene and functionalized graphene which leads to its enormous applications in energy storage devices, paints, coatings, biomedical devices, and hydrogels etc.

Contents

1. Introduction & literature Survey
2. Material & experimental techniques
3. Synthesis and characterization of graphene oxide and reduced graphene oxide from graphene
4. Physical, structural and morphological characterization of graphene, graphene oxide and reduced graphene oxide reinforced PVA nanocomposites
5. Mechanical and thermal characterization of graphene, graphene oxide and reduced graphene oxide reinforced

pvabionanocomposites 6. Rheological characterization of graphene, graphene oxide and reduced graphene oxide reinforced pvabionanocomposites. 7. Summary, Conclusions and future scope. List of publication.

02. BORUAH (Jiten)

Application Specific Design of Photonic Crystal Fibers, Waveguides and Devices.

Supervisor : Prof. R. K. Sinha

Th 24205

*Abstract
(Not Verified)*

Photonic structures in Photonic Crystals (PhC) are optical analogue of electronic structures designed for use in photonic circuits and envisaged to replace electronic circuits in near future. In this thesis, investigation of photonic structures less sensitive to environmental fluctuations and design of PhC and point defect cavity using temperature resilient material Silicon Carbide (SiC) for 1.55 μm have been reported. The effect of temperature on different parameters of the PhC and cavity have been studied and compared with that of Si PhC and cavity using plane wave expansion and finite difference time domain methods. The SiC photonic structures found to sustain high temperature and power transmission not possible in Si photonic structures leading to predict an era of silicon carbide power photonics analogous to silicon carbide power electronics. The most significant application of PhC is the design of Photonic Crystal Fiber (PCF) waveguide with confinement characteristics not possible in optical fiber. In this thesis, the application specific designs of following PCF have been proposed and their propagation characteristics investigated by employing Finite Element Method and MATLAB. The Fluoropolymer PCF has been designed for use in long distance telecommunication and sensing in terahertz region. The W-type PCFs have more power coupling compared to conventional PCF, bend insensitive and highly nonlinear and can be used for large mode area (LMA) fiber design, fiber to the home and nonlinear applications in visible and near infrared region. The cladding doped LMA W-type PCFs are of low confinement and bend losses, birefringent and sensitive at 1.55 μm and predicted for applications in telecommunication and sensing. The Ga-Sb-S based chalcogenide glass PCF has been studied for the first time since the inception of the novel material Ga-Sb-S for wavelength range 0.8 μm to 14 μm and can find nonlinear mid-infrared applications in fiber lasers, generation of supercontinuum and slow light.

Contents

1. Introduction. 2. Demonstration of temperature resilient properties of 2D silicon carbide photonic crystal structures and cavity modes 3. Characterization of fluoropolymer photonic crystal fiber for THz regime 4. Temperature dependent bending loss characteristics of W-type photonic crystal fibers: Design and analysis 5. Design and analyses of cladding doped large mode area W-type photonic crystal fiber for high power delivery devices and sensing applications 6. Low bend loss photonic fiber in Ga-Sb-S based chalcogenide glass nonlinear applications: Design and analysis 7. Summary and future scope of research work. References.

03. GUPTA (Bhawna)

Study of Propagation of Discontinuous Waves in Gas Dynamics

Supervisor : Prof. Jasobanta Jena

Th 24179

Abstract
(Not Verified)

The thesis consists of five chapters. The first chapter presents a brief introduction of the research topic. The second chapter deals with the propagation of one-dimensional shock waves of arbitrary strength through an inviscid, one dimensional, spherically symmetric, self-gravitating interstellar gas cloud. An infinite set of transport equations is obtained. A truncation procedure is used to put an end to infinite hierarchy of equations. The first three truncated equations describing shock strength and the induced discontinuities are considered and used to study the growth and decay of shock waves. The third chapter considers the problem of the motion of waves leading to shocks in an ideal gas under the influence of magnetic pressure using singular surface theory. Bernoulli type transport equation depicting the nonlinear coupling between the induced discontinuity and flow behind is obtained. The effects of van der Waals excluded volume and magnetic pressure are observed. The fourth chapter deals with the analysis of the disturbances propagating through an unsteady, inviscid nonideal gas in a magnetic field. Various cases keeping the shock amplitude as finite, small and not so small are studied using the technique of relatively undistorted waves. Further an asymptotic solution valid up to first and second-order approximations is found using the theory of weakly nonlinear geometrical optics and the effects of wave front configuration, nonideal parameter and magnetic pressure on the formation and subsequent propagation of shock waves are considered. The fifth chapter seeks an asymptotic solution to a system of equations governing one dimensional, unsteady, axisymmetric motion of a transient pinched plasma in the far field. The result is an inviscid Burger's equation. This equation is solved analytically. The results obtained by the same are compared with those obtained by numerical methods.

Contents

1. Introduction 2. Kinematics of spherical waves in interstellar gas clouds 3. On singular theory to study steepening of waves in non ideal magnetogas dynamics 4. Propagation and interaction of waves in non ideal magnetogas dynamics 5. Far field behaviour of waves in transient pinched plasma. Bibliography.

04. MALIK (Neha)
Convergence Estimates For Certain Linear Positive Operators.
Supervisor : Prof. Vijay Gupta
Th 24181

Abstract
(Verified)

The thesis deals with the convergence estimates for certain linear positive operators of summation integral type. In this work, generalized versions of some recent operators are studied and their approximation properties are investigated. The errors in approximation for these operators caused due to functional norm or point-wise convergence are taken care of. This is the importance of discussing these hybrid linear positive operators. The thesis is mainly divided into six chapters. Chapter 1 introduces the concepts of linear positive operators, which are relevant to our further investigations. In Chapter 2, we study the approximation properties of the generalized Lupas-Szász type operators, wherein the basis function contains Paltanea's weights. We provide an alternate approach to obtain the moments using the concept of moment generating function and then, certain well-known direct results are shown to follow easily. Chapter 3 incorporates the studies related to the modified Baskakov-Szász operators involving two nonnegative parameters. We introduce hybrid Durrmeyer type operators by taking the weights of Jain basis function. It is observed that by considering Jain basis function in integral,

moments estimation of higher order becomes difficult, but we overcame this difficulty and estimated few moments. Chapter 4 deals with the approximation properties of the genuine Baskakov type operators based on certain parameters. We establish some direct estimates along with some convergence estimates in L_p norm. In Chapter 5, the genuine Polya-Durrmeyer type operators in the complex domain are studied. The sepolynomials preserve constant as well as linear functions. For the approximation of such analytic functions in a certain disk, an upper estimate, asymptotic formula and exact order are estimated. Last chapter provides the convergence behaviour of two (p,q) -variants of Durrmeyer type operators, viz. (p,q) -Baskakov-Beta and (p,q) -Bernstein-Durrmeyer operators. We obtain a relation between (p,q) -Beta and (p,q) -Gamma functions, and establish some approximation properties along with graphical comparison for different parameters.

Contents

1. Introduction 2. Convergence estimates for generalized lupas – Szasz type operators
 3. Convergence estimates for mixed hybrid durrmeyer type operators 4. Convergence estimates for baskakov – durrmeyer operators 5. Convergence estimates for complex polya genuine durrmeyer type operators 6. Convergence estimates for (p,q) – durrmeyer type operators. Future work Plans. Referecnces.

05. MOHANTY (Pallavi)
Structure, Dynamics and Interactions of Focal Adhesion Kinase in Cardiac Hypertrophy.
 Supervisor : Dr.Sonika Bhatnagar
Th 24178

Abstract (Verified)

Cardiac hypertrophy is the thickening of heart muscle and is an adaptive change as seen in athlete's heart. Pathological cardiac hypertrophy (PAH) is an abnormal thickening of heart muscle due to high blood pressure and leads to heart failure. Literature review, pathway analysis and interaction analysis showed that the Focal adhesion kinase (FAK) is a critical molecule that mediates switching between the healthy and diseased heart condition. Phosphorylation is the key event in FAK activation. A normal FAK-Paxillin interaction leads to normal development in heart. Hyper activation occurs by phosphorylation at aberrant sites and allows FAK-Grb2 interaction leading to PAH. As, FAK phosphorylation was linked with its activation and hyper activation, three FAK forms were conceptualized. Molecular modeling of all three FAK forms were carried out using combination of homology modeling, threading, *ab initio* and domain assembly approach followed by 100ns classical molecular dynamic simulations. The models of full FAK in its various forms provided a structural basis for FAK activity in health and disease. Hyperactive FAK showed disruption of the FAK-Paxillin binding site, thus disrupting the stabilized form. Targeted molecular dynamics of the FAT domain of FAK was further used to fetch the structural intermediate that showed competence for Grb2 interaction. The FAT intermediate obtained was docked with Grb2 in order to identify the structural features of their interaction. The FAT-Grb2 interface analysis was done to identify two pockets responsible for FAT binding in Grb2-SH2 domain. Pharmacophore modeling, virtual screening in combination with absorption, distribution, metabolism, excretion and toxicity predictions techniques were used to propose high affinity and selective drug-like molecules against FAT-Grb2 interaction that can act as a therapeutic candidate for PAH.

Contents

1. Introduction and literature review 2. Material and methods 3. Focal Adhesion Kinase Phosphorylation 4. Targeted molecular dynamics to determine 5. In silico screening of high affinity and selective ligands against Grb2 – SH2 domain as therapeutic candidate for PAH 6. Conclusion and future scope of work 7. List of Publication 8. Bibliography.

06. SINGLA (Rajeev Kumar)
Phytoconstituents of *Cocos nucifera* Linn. Endocarp: Isolation, Characterization & their Therapeutic Properties.
Supervisor : Prof. Ashok Kumar Dubey
Th 24176

Abstract
(Verified)

Cocos nucifera's shell has multifarious therapeutic potential. To the best of our knowledge, its phytoconstituents profile was not known. So, the objective was to initiate this characterization of this plant part by isolating phytoconstituents and structurally and functionally characterize them. Phytochemical profiling indicated the diverse class of compounds present in ethanolic extract and shell oil. GCMS of ethanolic extract indicated the probability of having myristic acid, syringaldehyde, eugenol, vanillin, 2,4-di-tert-butylphenol, lauric acid, methyl palmitate, and γ -sitosterol. GRIP docking studies of these molecules were done against porcine pancreatic α -amylase. γ -sitosterol had shown the highest affinity with hydroxyl oxygen atom as the pharmacophore. DMPK and toxicological predictions were done using StarDrop. Further, correlation between dock score with α -amylase and ADME parameters revealed that LogS is inversely proportional to the dock score and this is vice versa in case of 2C9 pKi and hERG pIC50. The ethanolic extract was further fractionated by using column chromatography. Starch iodine plate assay and DNS-based α -amylase inhibitory assays indicated that Fractions, designated as B and C, were the best among tested fractions. Fraction B was further fractionated using different solvents as well as by TLC-based separation, which yielded a sub-fraction with single band. Analysis of spectral data indicated that it is novel ketofatty acid, nuciferoic acid. Nuciferoic acid has displayed moderate inhibition of hyaluronidase enzyme. It was docked in 10 cavities of hyaluronidase and compared with its substrate hyaluronic acid. Cavity 1 and 4 could be probable site on hyaluronidase for nuciferoic acid. Further, the shell oil was screened for the antimicrobial activity against bacterial strains *S. aureus*, *E. coli*, *P. aeruginosa* and was found to exert inhibitory effect on these test strains at a concentration as low as 6.5 μ g/well. Using liquid-liquid extraction and flash chromatography, one molecule was isolated from shell oil with 82.27% purity.

Contents

1. Introduction and Objectives 2. Literature review 3. Materials and methods 4. Result and discussion 5. Summary 6. Conclusion 7. Bibliography. Appendix.

07. SHARMA (Kanishka)
Effect of Long-term meditation on Human Attention Networks : Study of Electrophysiological Indices.
Supervisor : Prof. A. K. Dubey
Th 24180

Abstract
(Verified)

Meditation and related practices are beneficial for overall health. Its effects were seen on the neuronal system and cognitive indices. Different types of meditation were examined for their effects on the human nervous system. Brahma-Kumaris Rajayoga meditation is versatile, easy

to practice and followed by more than a million people world- wide. Neurophysiological effects of Rajayoga meditation on attention networks and related brain structures have been explored in the present study. Long-term meditators with regular ten years of meditation experience and control subjects as meditation naïve/having no experience practicing meditation were selected for the study. Electroencephalography (EEG) and diffusion tensor imaging(DTI) were utilized to examine chronic changes in human brain. Performance in computer-based Attention Network Task (ANT) was recorded. Accuracy, overall reaction time and index of attention components (alerting, orienting and executive attention) were calculated. MATLAB was used for calculating alpha and theta band powers and, alpha asymmetry. Asymmetry is an informative factor for task-based cognitive processing and attention networks. Fractional anisotropy (FA) and mean diffusivity (MD) were quantified from DTI images. Findings revealed micro/macro-structural changes in the white matter of long-term meditators due to the regular practice of meditation. Significant differences in reaction time and accuracy indicated better attention resources in long term meditators. Lower frequency (alpha: 8-13 Hz and theta: 4-7 Hz) band power and asymmetryindex were high in the frontal and parietal cortex. Brain networks for regulation of attention and emotions might be affected positively due to meditation. Increased FA and reduced MD were found in different regions of the corpus callosum (CC) as well as in other white matter tracts. Strongmyelination may provide efficient neural transmission. Overall findings suggest that Rajayogameditation may prove to be an effective strategy to enhance attention control and may help inpreserving white matter in the human brain.

Contents

1. Introduction and objectives 2. Review of Literature 3.Long term meditation and lower frequency EEG dynamics 4.Properties of white matter fiber tracts in long term meditators 5.Resting state network in long term meditators 6. Psychometric analysis of attention networks 7. Summary.Bibliography.List of publication.Reprints of Publications.