CHAPTER 46

PHYSICS AND ASTROPHYSICS

Doctoral Theses

01. BHATT (Vijay)
Quantum Optical Properties of Hybrid Semiconductor Systems: Applications in Optical Switching and Nonlinear Phenomenon.
Supervisors: Prof. Pradip Kumar Jha and Prof. A. Bhattacherjee
Th 28446

Abstract

According to recent research, nanostructures such as quantum dots are effective systems for addressing the challenges posed by Moore`s law, because of their narrow linewidths and the capability to develop tunable quantum devices. In cavity electrodynamics, an optical semiconductor microcavity coupled with an emitter is used to investigate the interaction between light and matter. My Ph.D. research focused on studying the quantum optical characteristics of hybrid semiconductor systems underlying the basic principle phenomenon with their applications in device development. The first chapter gives a basic introduction to the physical phenomena related to the light-matter interaction. Chapter two describes the mathematical methods used in this thesis to address the research problem. Many methodologies and strategies are used to understand the system`s dynamics. Chapter three deals with the system of photonic crystal cavity containing double quantum dot and Kerr nonlinear medium. In chapter four, we studied the cavity quantum electrodynamic system embedded with two coupled quantum dots (QDs) and a Kerr nonlinear medium. We studied Four-Wave Mixing (FWM) and Normal Mode Splitting (NMS), which is a significant manifestation of coupled two QDs cavity system is observed in the form of NMS, due to fast energy exchange among all degrees of freedom. These results suggest the suitability of the proposed system for quantum information processing. In Chapter Five the hybrid optomechanical system comprises an ensemble of N number of quantum dots (QDs) in the presence of third order nonlinear $\chi^{(3)}$ medium investigated theoretically. Utilizing the Holstein-Primakoff (H-P) transformation formalism, we study the bistability and absorption of the system analytically and numerically. Results show that the system is well-suited for developing next-generation optoelectronic devices. Chapter six contains the conclusions of my research as well as a possible outline of the current work`s future aspects.

Contents

1. Introduction 2. Methodology 3. Optical response in a double quantum dot molecule inside a nonlinear photonic crystal cavity 4. Normal mode splitting and Four-wave mixing in Kerr-nonlinear optical system containing coupled double quantum dot 5. Holstein–Primakoff (H-P) Approach to Determine the Optical Response of Hybrid Optomechanical system containing Multiple Quantum Dots 6. Conclusions. Bibliography and Appendix.

02. CHETNA
Beyond Standard Model Interactions of Charged Leptons.
Supervisor: Prof. Surendra Kumar Dhaka
Th 28447

Abstract

Delhi, one of the most polluted cities globally, serves as a critical case study for examining the dynamics of particulate matter (PM2.5 and PM10), which significantly affects health, visibility, and climate. Existing research predominantly focuses on short-term datasets or a limited number of air quality monitoring stations, with little attention given to the long-term influence of meteorology. This Ph.D. thesis addresses these gaps by investigating the temporal variability of particulate matter (PM2.5 and PM10) in Delhi from 2007 to 2022 across multiple timescales daily, monthly, seasonal, annual, and inter-annual while exploring its relationship with meteorological factors. Using robust non-parametric statistical techniques, including the Mann-Kendall test, Theil-Sen slope estimator, and smooth-trends derived from Generalized Additive Modelling (GAM), this study analyzes long-term trends in PM2.5, PM10, and key meteorological parameters. A unique aspect of this research is the examination of the COVID-19 lockdown, which provided an unprecedented opportunity to observe the substantial reduction in pollution levels due to the sudden cessation of anthropogenic activities. The findings reveal how specific meteorological conditions such as low temperatures, calm winds, and high relative humidity contributed to the formation of haze events and sharp increases in PM2.5 concentrations during morning hours, underscoring the interaction between baseline pollution and local meteorology. Furthermore, the study decodes the monthly, seasonal, inter-annual variability, and long-term trends in PM2.5 (2007–2022) and PM10 (2015–2022), offering a multi-year comprehensive assessment of both meteorology-adjusted and unadjusted trends in PM2.5 using the AirGAM statistical model. The research highlights gradual air quality improvements due to policy interventions and explores the non-linear relationships between particulate matter and meteorological factors. Overall, this work advances the understanding of particulate pollution variability and its meteorological drivers, providing insights for developing more effective air quality mitigation strategies.

Contents

03. DAHIYA (Brijender)
Field Induced Effects on Information Theoric Measures.
Supervisor: Prof. Poonam Silotia
Th 28448

Abstract

The work presented in the thesis entitled “Field induced Effects on Information Theoric Measures” mainly focuses on the study of information theoric measures like Shannon entropy in position and momentum space, and the total Shannon entropy, Rényi entropy, Tsallis entropy, Kullback–Leibler (KL) distance, Onicescu information energy, and Lupez-Ruiz, Manicini & Calbet (LMC) complexity in the presence of external fields. The system under study in the thesis is taken (a) Spherically confined H-atom (CHA), (b) H-atom confined in fullerene, (c) Particle in a Spherical Box (PISB), and (d) free H-atom (FHA) interacting with the laser field These information theoric measures are calculated for the free and the confined systems. The findings align well with the literature for field-free conditions. The interplay between confinement and external fields is highlighted. For tight confinement, CHA behaviour approaches the results of PISB. The total Shannon entropy in PISB remains independent of the confining radius, whereas for CHA, Coulomb interaction induces minima or maxima. An increase in the electric field causes the interaction variations to shift towards a lower confining radius. The thesis contains six chapters: Chapter 1 covers the introduction, literature review, and applications in diverse fields. Chapter 2 discusses mathematical tools used in the study. Chapter 3 examines the electric field effects on the Shannon entropy of CHA and the H-atom confined in a fullerene cage. Chapter 4 examines PISB, and various information theoric measures are studied for field-free and field-assisted conditions. Chapter 5 investigates the interaction of FHA with a laser field, revealing the role of Shannon entropy in avoided crossings. The exchange of Shannon entropy at avoided crossings makes Shannon entropy an indicator of avoided crossings. With an increase in laser amplitude, the AC Stark effects are observed. Chapter 6 summarizes findings and future perspectives.

Contents

04. DEEPAK KUMAR

Realization of Landslide Early Warning System Based on Acoustic Emission Technology.

Supervisors: Prof. Ajit K. Mahapatro and Dr. Sushil Kumar Singh

Th 28450

Abstract

Landslide disasters pose significant risk to human lives and infrastructure, highlighting the need for a reliable landslide early warning system (LEWS). This Ph.D. thesis is focused on utilizing acoustic emission (AE) technology for real-time monitoring of landslide prone slopes and the development of robust LEWS. The research aimed to optimize the active waveguide system (AWS) for slope monitoring, correlate AE characteristics of AWS with slope deformation dynamics, standardize slope deformation dynamics for LEWS, and design an AE based slope monitoring system capable of issuing alerts when the risk of slope failure becomes critical. Laboratory AE calibration of AWS models was performed to establish a threshold deformation velocity of 1 mm/min. Validation studies were performed using artificial soil slopes under controlled failure conditions, confirming the threshold velocity`s reliability for early warnings. Critical AWS parameters, including waveguide diameter, backfill material, and flexible membranes, were optimized for their AE behavior during slope deformations. AE timing parameters of hit definition time, hit lockout time, and peak definition time were also optimized to capture accurate signatures of AE signals. To design and develop a generalized LEWS, distinct landslide velocity scales inspired by Varnes' classification were proposed and quantified through AE signal parameter analysis under varying deformation rates. Soil shear deformation dynamics were further investigated using large-scale soil shear tests, establishing correlations between AE characteristics and landslide velocity scales. Additionally, AE technology was employed to assess shear zone depths within slopes, demonstrating its potential for precise localization, landslide susceptibility mapping, and hazard mitigation. The thesis concludes with the design of an integrated sensor system for LEWS, combining AE technology with rainfall measurements from automatic weather stations for comprehensive slope instability assessment. This system generates real-time alerts based on AE-derived deformation metrics and rainfall-induced instability, enhancing the reliability of early warning alerts for landslide risk reduction.

Contents

05. DISHU (Dawra)

Study of Photoionization of Complex ions useful in Astrophysics & Plasma Physics.

Supervisors: Prof. Avnindra Kumar Singh and Prof. Anil K. Pradhan

Th 28449

Abstract

Atomic physics is an essential and basic field of physics that deals with the structure of atoms, their mutual interaction and their dynamics. Spectroscopy has been the enabling tool for research in various branches of physics such as plasma physics, atomic physics, X-ray astronomy, and fundamental science. A detailed analysis of the spectra contains tremendous information regarding the density, temperature and composition of the remote source. Therefore, atomic data such as energies, transition wavelengths, transition probabilities, oscillator strengths and line strengths are required for the modeling and diagnostics of astrophysical and laboratory plasmas. Accurate estimates of transition probabilities are important for the experimental identification of spectra, but the experimental determination of probabilities is difficult, and one has to rely on the accurate theoretical calculations. For the past few decades, theoretical atomic physicists have done great efforts for the development of various methods such as the configuration interaction method (CIV3), multiconfiguration Dirac-Fock (MCDF) method and R-matrix technique for computation of vast amount of theoretical atomic data. In this thesis, we have

presented atomic structure and photoionization calculations for highly charged ions. We have calculated level energies, oscillator strengths and transition probabilities for Na-like Cu XIX ion using the configuration interaction (CI) method CIV3. We have also presented excitation energies, radiative decay rates, oscillator strengths, line strengths and lifetimes for Na-like Se XXIV ion using the multiconfiguration Dirac-Fock (MCDF) method. Moreover, we have employed the state-of-the-art R-matrix technique for calculating photoionization cross sections of Ne-like Co XVIII and Na-like Ni XVIII ions. Further, the plasma screening effect on the photoionization of H-like O7+ ion is studied in strongly coupled plasma within the framework of relativistic configuration interaction technique. The present results will be beneficial for the interpretation of spectra observed in a variety of astrophysical and laboratory plasmas.

Contents

1. Introduction 2. Configuration Interaction Calculations of Energy Levels and Radiative Data in Na-like Cu XIX 3. Multiconfiguration Dirac-Fock Energies and Transition Rates for Cu XIX and Se XXIV 4. Photoionization Cross Section Calculations for Complex Ions 5. Influence of Strongly Coupled Plasma Environment on Photoionization of H-like O^{7+} ion 6. In-beam x-ray Spectroscopy and Shel Model Calculation in 86Rb 7. Concluding Remarks and Reprints of the Research Papers.

06. GOGOI (Pragjyotish Bhuyan)
Hopf Bifurcation in High-Dimensional Nonlinear Systems.
Supervisor: Prof. Awadhesh Prasad
Th 28451

Abstract

We study the phenomenon of Hopf bifurcation in high-dimensional nonlinear systems, which can either be generalisations of their low-dimensional counterparts or can appear in the form of coupled low-dimensional oscillators. We first present a D-dimensional generalisation of the normal form for Hopf bifurcation described by the Stuart-Landau model, using Clifford`s geometric algebra. We show that in this generalised picture, Hopf bifurcation mediates the transition between an equilibrium state and an oscillatory state which is characterised by extreme multistability and can either be periodic or quasiperiodic depending on the parameters. The exact solvability of the model facilitates a complete description of the model. We then study the collective behaviour of two D-dimensional oscillators and analyse how the presence of two additional parameters in this case, namely the coupling strength and the quantified dissimilarity between the two oscillators, modulates the dynamics, and affects the appearance of Hopf bifurcation. Lastly, we describe a system of nonlinear oscillators whose interaction is modulated by the extent of similarity of their state variables, quantified using measures such as the distance between the oscillators in phase-space. For a system of coupled Stuart-Landau oscillators, we show that the individual oscillators, initially confined to inhomogeneous limit cycles, asymptotically approach two different fixed points as the bifurcation parameter is increased, outlining a novel form of Hopf bifurcation from oscillations to oscillation death.

Contents

1. Introduction 2. Hopf bifurcation described by a generalised Stuart-landau system 3. Hopf bifurcation in two coupled generalised Stuart-Landau oscillators 4. Hopf bifurcation in nonlinear oscillators with similarity-dependent coupling 5. Summary and discussions. Bibliography.

07. JHARWAL (Swati)
Investigation on Structural and Magnetic Properties of Lanthanum Based Double Perovskites.
Supervisors: Prof. Vivek Kumar Verma and Dr. Arvind Kumar
Th 28740

Abstract

Perovskite materials have been at the forefront of the materials science research in last few decades owing to their diverse physical properties exhibited by them. After the discovery of GMR by nobel laureates Albert Fert and Peter Grunberg, there has been a complete metamorphosis in the field of memory devices. With the advent of information technology, the need for efficient, smaller and faster devices is increasing. The very few room temperature multiferroic materials are perovskites and has the potential to revolutionise the future electronic industry. Magnetoresistance is a particularly interesting property shown by perovskites which has multiple applications. From the detailed literature survey, lanthanum based double perovskites are selected as the compound for present investigations. The synthesis method of double perovskite La2CoFeO6 has been optimised by varying the synthesis techniques and synthesis parameters. Further to enhance the magnetic properties of double perovskite La2CoFeO6, the effect of A-site and B-site substitutions on the structural and magnetic properties of La2CoFeO6 have been studied in details. X-ray diffraction, FTIR and Raman spectroscopy techniques have been employed for detailed structural investigations. FESEM/TEM/SEM were used to analyse the morphological properties of prepared samples. Field dependent and temperature dependent magnetisation properties have been studied in light of the core level XPS spectrum of the cations to understand the nature of magnetic behaviour and magnetic transitions exhibited by the prepared compounds. The results revealed that the magnetisation of the double perovskite La2CoFeO6 can be enhanced by reducing the particle size. The transition temperature of La2CoFeO6 was tuned to near room temperature by varying the Fe/Co ratio making it a strong candidate for spintronic applications. Sr substitutions at La site lead to improved magnetic properties and can be further explored for potential applications. This study provides insights into the magnetic properties of the lanthanum based double perovskites for their potential applications in spintronic devices.

Contents

08. KADIAN (Ankit)
Charge Transfer Studies in Metal Oxide-Based Heterostructure Photocatalysts Using Synchrotron Radiation.
Supervisor: Prof. S. Annapoorni
Th 28452

Abstract

Rapid industrialization and urbanization have raised environmental challenges due to water and other pollution hampering our pursuit of sustainable development. Photocatalysis has emerged as a promising sustainable solution for environmental remediation and water treatment due to its pollutant degradation ability with minimum energy infrastructure. This thesis explores the synthesis, characterisation, and photocatalytic performance of ZnO, Co_3O_4, and their graphene-based composites. The primary focus is on understanding the defect states, charge transfer mechanisms, and structural modifications that enhance photocatalytic activity. The study comprehensively discusses fundamentals of photocatalysis, emphasizing the significance of material selection. Facile alkaline-precipitate and chemical colloidal refluxing synthesis routes are employed to obtain desired materials. Characterisation techniques such as X-ray diffraction (XRD), UV-Visible spectroscopy, photoluminescence spectroscopy, electron microscopy, and synchrotron radiation-based advance experimental methods are utilized to analyze the structural, optical, morphological, and electronic properties of the synthesized materials. The investigation delves into the defect states of nano-sized peanut-shaped ZnO (N-ZnO) and micron-sized hexagonal rod ZnO (M-ZnO) using synchrotron-XRD and X-ray absorption spectroscopy (XAS) coupled with X-ray excited optical luminescence (XEOL). Their photocatalytic degradation of rhodamine B dye is evaluated. Furthermore, ZnO/graphene composites are studied for methylene blue degradation, with a focus on band structure modifications and defect analysis using low-temperature photoluminescence. The role of the carbon network in cobalt oxide-graphene and cobalt oxide-graphene oxide nanocomposites is explored through structural and charge transfer analysis using XRD, electron microscopy, and XAS. Photocatalytic degradation of phenol under UV-visible light is correlated with in-situ XAS studies to elucidate charge transfer dynamics. Additionally, cobalt-modified ZnO nanocomposites are investigated for their potential as UV filters in sunscreens, demonstrating reduced reactive oxygen species (ROS) generation and improved sun protection factor performance. This thesis provides insights into the rational design of metal oxide-graphene-based photocatalysts and their applications in mitigating water pollution.

Contents

09. KAUR (Manjeet)
Physics of Early Universe with Inflation and Bounce.
Supervisors: Prof. Debajyoti Choudhury and Prof. T. R. Seshadri
Th 28453

Abstract

The Standard model of Cosmology, based on the Big Bang theory, successfully describes broad aspects of the evolution of the Universe. However, it faces several unresolved issues, such as the horizon, flatness, and singularity problems. To resolve these issues, two main alternatives have emerged: the inflationary paradigm

and bouncing cosmology. The inflationary paradigm suggests an early phase of accelerated expansion, smoothing out initial irregularities and explaining the uniformity of the Cosmic Microwave Background Radiation. Despite its successes, it faces degeneracy problem (multiple viable models) and the initial singularity problem. Bouncing cosmology proposes a contracting phase followed by a non-singular bounce leading to expansion. This model is also capable of addressing homogeneity and isotropy of the Universe but requires null energy condition violation, leading to potential instabilities. Thus, the inflationary paradigm suffers from theoretical inconsistencies, and the bouncing paradigm suffers from both theoretical as well as observational inconsistencies. In this thesis, we use two different approaches to avert these inconsistencies. The first approach focuses on a hybrid Cosmological model obtained by combining bouncing and inflationary phases, where a pre-inflationary bounce transits smoothly into a viable inflationary phase. This model uses two minimally coupled scalar fields within the framework of Einstein-Hilbert gravity, with one field engineering the required null energy condition violation to achieve a bounce. A non-trivial coupling between the fields helps mitigate potential ghost instabilities, ensuring stability and consistency with observational data. The second approach focuses on improving the accuracy of theoretical predictions for key observables corresponding to inflationary models by employing a novel phase-space variable reparameterization. This method provides a unified description of the evolution of the Universe, bridging the gap between slow-roll inflation and the oscillatory phase. These refined predictions allow for tighter constraints on inflationary parameters and an accuracy comparable to that expected in future observational data.

Contents

10. KIRTEE KUMAR

Some Aspects of Information Theory for Spherically Symmetric Confined Systems and Coupled Quantum Systems.

Supervisors: Prof. Vinod Prasad and Prof. Poonam Silotia

Th 28454

Abstract

This thesis deals with a detailed study of confined quantum systems using concepts from information theory, with a special focus on entropy-based and correlation-based measures. The main aim is to understand how spatial confinement affects the behavior of different information-theoretic tools, like Shannon entropy, mutual information, and statistical correlation coefficients of quantum systems. These measures are employed to study the localization and delocalization of wavefunctions and to evaluate the uncertainty relations more effectively than the conventional Heisenberg principle. The beginning of the work is devoted to examining hydrogen atoms placed under spatial confinement using modified Hulthen and Hellmann-type screening potentials. The Schrödinger equation is solved numerically using the finite difference method, and computing the energy spectra, radial distributions, and entropy measures. The results show how confinement and screening parameters influence entropy and uncertainty. The study extends to Rydberg atoms, which are known for their highly excited and extended quantum states, to analyze their entropy behavior in both free and confined conditions. It is observed that Shannon entropy varies with atomic number and confinement radius, which helps in understanding the localization and delocalization features of highly excited states. The results also show that entropy-based uncertainty relations are better than the Heisenberg uncertainty principle in such systems. In the final part of the thesis, we study the quantum correlation in coupled systems. Two important models are considered: the Moshinsky atom, which allows an exact solution, and a coupled double-well system described by Razavy`s hyperbolic potential. These models are used to explore both statistical and entropic correlations. Various quantities such as Shannon entropy, mutual information, and statistical correlation coefficients are computed to study the behaviour of these coupled systems under confinement. Additionally, entanglement measures like von Neumann and linear entropy are used to quantify quantum correlation. Overall, the work shows that information theory provides a deeper understanding of quantum properties under confinement and gives valuable insights for applications in quantum technologies, including quantum computing, quantum communication, and high-pressure physics.

Contents

11. MAHARANA (Suvam)
Taming Hierarchies with the Clockwork Mechanism: A Theoretical and Phenomenological Study.
Supervisor: Prof. Debajyoti Choudhury
Th 28463

Abstract

Phenomenological models in particle physics often assume hierarchical mass scales and/or couplings in order to explain low-energy phenomena. For instance, the Standard Model (SM) presupposes hierarchical Yukawa couplings to explain the observed fermion masses. Even in scenarios beyond the SM that contain new light particles (such as axions, dark photon, etc.), the pertinent couplings of the latter with the SM sector are typically constrained to be small by experimental observations. While such hierarchies may appear tenable from a strictly phenomenological standpoint, an investigation of their possibly more fundamental origins is warranted so as to fully understand the high-energy behaviour of the theory. In other words, one ought to identify an underlying mechanism which can naturally generate the required hierarchies in a theory without invoking ad hoc fine-tunings in the parameters. To this end, the clockwork paradigm provides an interesting framework whereby large hierarchies can be generated within theories containing O(1) parameter values. The mechanism employs theory spaces defined by multiple copies of a field interacting through near-neighbour couplings such that the lightest state is localized near one end of the lattice whereas the heavier modes are nearly delocalized. The thesis presents a theoretical study of the clockwork mechanism as well as explores some of its phenomenological applications. On the theoretical side, we extend the original formalism of the mechanism on a one-dimensional theory space lattice to a periodic lattice and describe the new features that emerge. We further identify the correspondence of such a theory with a linear dilaton theory of gravity in five spacetime dimensions. As for the phenomenological applications, we study models for a KSVZ-like QCD axion augmented by a one- and a two-dimensional clockwork lattice, wherein a large effective decay constant for the light axion is automatically generated through the clockwork mechanism. Interestingly, the associated heavy pseudoscalars act as axion-like particles (ALPs) which can, in principle, have masses and decay constants that are accessible at collider experiments. We identify interesting benchmarks in both the one- and two-dimensional setups for which the ALPs may be visible at the hadron colliders (such as the currently operating LHC and the forthcoming HL-LHC) with unique signatures. On the other hand, the two-dimensional model also accommodates long-lived ALPs which may be detected in some of the upcoming displaced-vertex detector experiments. Furthermore, we also demonstrate the possibility of achieving baryogengesis via leptogenesis within a clockwork model for neutrino masses with anarchic textures of the Yukawa matrices containing nearly O(1) elements. We conclude by commenting on the apparent shortcomings of the formalism as well as on the possible future directions.

Contents

12. MOTLA (Akanksha)
Fabrication of Metal/Metal– Oxide Plasmonic Based Surface Enhanced Raman Spectroscopy (SERS) Platforms for Detection of Organic Dyes.
Supervisor: Prof. S. Annapoorni
Th 28455

Abstract

This thesis focuses on the fabrication of surface enhanced Raman spectroscopy (SERS) substrates using hybrid structures of metal oxide and noble metals for the detection of organic dyes. Organic dyes are known to be major environment pollutants and are also used as coloring agents in food products, which can be harmful to living organisms. SERS is an effective technique for detecting trace quantities of organic dyes more efficiently and swiftly. Chapter 1 provides the motivation behind this research and gives an introduction to various organic dyes and detection techniques. It discusses the Raman spectroscopy in detail, highlighting its limitations and the need for modification to enhance its detection sensitivity. Further, the chapter describes the mechanism involved in SERS through an extensive review of literature study supporting the selection of material and emphasizing the necessity for both rigid and flexible SERS substrates. Chapter 2 discusses the principles and methodologies of the various material synthesis techniques and characterization techniques used in the fabrication of effective SERS substrates. Chapter 3 reports the chemical synthesis of hybridized silver (Ag) nanoparticles onto zinc oxide (ZnO) nanorods to create SERS substrates on rigid silicon (Si) platforms. The presence of varied morphology and the plasmonic entity (Ag), enhances the SERS sensitivity tested for low concentrations of organic dyes, rhodamine B (RhB) and methyl orange. Chapter 4 investigates ZnO sheet like structures deposited using thermal evaporation and further modified through ex-situ annealing in various environments. These modified ZnO substrates were examined for their potential SERS application, for the detection of organic dyes. However, these lacked the required sensitivity in the absence of a plasmonic entity, which is a key requirement for SERS. Chapter 5 further reports the fabrication of co-sputtered Ag-ZnO on a rigid quartz platform. The plasmonic properties were tuned by varying the Ag deposition power in the fabricated samples. A post deposition

annealing further modified the surface properties of the substrates for enhanced SERS sensitivity of RhB detection. However, in the real world, the analyte molecules are found on rough or irregular surfaces. Hence, a quick and efficient detection is possible only by using flexible substrates. Chapter 6 explores gold (Au) deposited on flexible platforms of polyethylene terephthalate (PET) and indium tin oxide (ITO) coated PET using thermal evaporation. The Au surfaces on PET and ITO-PET were then modified using a 10 keV Ar+ ions, using a tabletop accelerator. The emergence of nanostructures on the surface facilitated multiple detections of RhB and PET molecules. Chapter 7 summarizes the experimental investigations conducted and provides an overview of the future prospects for this research.

Contents

13. PRAJAPATI (Vivek)

Study of Substrate-induced Graphene Superlattice: Valley Conductance, Reflection Probabilities and Thermodynamic Properties with Uniform Magnetic Field.

Supervisor: Prof. Nivedita Deo

Th 28456

Abstract

Graphene, a single layer of carbon atoms arranged in a hexagonal lattice, has emerged as a material of exceptional interest due to its remarkable electronic and thermal properties. The unique characteristics of graphene have paved the way for investigating its behavior in structured environments, such as graphene super-lattices induced by periodic substrates. This study delves into a comprehensive exploration of the transport and thermodynamic properties of such graphene super-lattices, aiming to unravel the intricate interplay between structure, electronic transport phenomena, and thermodynamic behavior. In the domain of electronic transport, the study focuses on Dirac fermions within the substrate-induced graphene super-lattice. Utilizing a tight binding model, the energy band structure is meticulously characterized, and topological regions are classified based on the topological order parameter. A notable observation is the valley-switching phenomenon, where Dirac fermions, endowed with valley degree of freedom, exhibit both complete and partial reflection and transmission to the other valley under specific structural parameter regimes. The conductance of the system displays intriguing behavior, featuring peaks at each Dirac point. This conductance pattern is found to vary with structural parameters, leading to a nuanced understanding of the transport properties in graphene super-lattices. Simultaneously, the study extends its focus to the thermodynamic properties of substrate-induced graphene superlattice in the presence of a uniform magnetic field. Employing the zeta function approach, a rigorous derivation of the partition function is achieved, enabling the determination of a suite of thermodynamic functions. These include the Helmholtz free energy, total energy, specific heat capacity, and entropy. The investigation encompasses three distinct cases related

to the sublattice potential, shedding light on the versatility of the system's thermodynamic response. Importantly, the study establishes the validation of the Dulong-Petit law across all cases in the high temperature limit, providing insights into the thermal behavior of the graphene super-lattice.

Contents

14. RAKHI KUMARI
Random Matrix and Network Analysis of Protein Families.
Supervisor: Prof. Nivedita Deo
Th 28457

Abstract

Proteins are vital for almost all biochemical and cellular processes. Although there is an enormous growth in the protein sequence data, the statistical characterization, structure, and function of many of these sequences are still unknown. In this thesis, we present a novel method for analyzing the structural organization of protein families by integrating random matrix theory (RMT) and network theory with the physiochemical properties of amino acids. This directly addresses the question of interaction patterns between amino acid residues that contribute to protein function. RMT distinguishes significant interactions between amino acids from background noise, pinpointing coevolving positions likely crucial for protein structure and function. Unlike previous methods that treat amino acids as mere characters, this property-based approach captures short and long-range correlations. The statistical and spectral analysis of the Pearson correlation matrices between positions of amino acids of seven protein families is performed and compared with the random Wishart matrix model results. A detailed analysis shows that the protein families significantly diverge from the Marchenko-Pastur distribution with many eigenvalues outside the Wishart lower and upper bound. The level spacing distribution is similar to the Gaussian orthogonal ensemble. Further, the number variance varies as a log of the system size indicates the presence of long-range correlations within the protein families. The eigenvector components of eigenvalue outside the RMT bound deviate from typical RMT observations, offering critical system information. We quantify the information content of each eigenvector using an entropic estimate, showing that the smallest eigenvectors are highly localized and informative. These eigenvectors form clusters of biologically and structurally significant positions. From the property-based correlation matrix we construct the threshold network and on a certain threshold, these crucial positions also emerge from the network analysis. This method enhances our understanding of protein evolution, interactions, and potential targets to modulate enzymatic actions.

Contents

15. RAVINDER KUMAR
Calculation of Excitation Energies, Transition Data, Collisional Ionization Cross Section and Rate Coefficient with Analysis of Line Intensity of Ag^{43+}, W^{64+} - W^{71+} and N^{+}.
Supervisor: Prof. Narendra Singh
Th 28458

Abstract

This thesis is composed of five chapters. In chapter 1, we have provided introductions relevant to the need and significance of atomic data in several fields. We have discussed the various theoretical methods, models, and online atomic databases. In Chapter 2, the atomic parameters of Ag XLIV (Be-like Ag) are examined and evaluated by implementing GRASP2K package with Multi-Configuration Dirac-Hartree-Fock (MCDHF) method. We have listed fine structure energy levels of the lowest 170 levels with radiative data for multipole moments such as electric dipole (E1), electric quadrupole (E2), magnetic dipole (M1) and magnetic quadrupole (M2) transitions that lie under the region of extreme ultraviolet (EUV) and soft X-ray (SXR) for Ag XLIV. We have compared our GRASP2K and FAC results with theoretical results available in literature for some levels. In chapter 3, electron impact ionization cross-sections of ground state are carried out for the energy range 20 keV to 1000 keV of final electrons, and Maxwellian rate coefficients for ground state are evaluated at the temperature range 20 keV to 300 keV for tungsten ions (W64+ to W71+) for fine structure levels of configurations containing n = 2 orbitals. To check the accuracy of calculated cross-sections and rate coefficients, a detailed comparison between results from different approximations—binary encounter dipole (BED), distorted wave (DW), and Coulomb Born exchange (CBE)—is presented. In Chapter 4, we discuss our calculations based on the collisional radiative model and multispectral line method to analyze spectra of N II in the visible range and determine the line intensity and flux ratio of spectral lines 476 nm and 528 nm, which have been observed in Cloud-to-Ground lightning spectra. Energy levels and lifetimes of 2p2, 2p3s, 2p3p, and 2p3d levels are presented, and found an extra ordinary lifetime of 3P1,2 states. In chapter 5, We have discussed the future work in atomic structure calculations, such as electron impact excitation, ionization, recombination, etc., plasma screening effect on fine structure energy levels; and line intensity and level population calculations on ions useful in plasma modelling.

Contents

16. RAWAT (Saraswati)
Synthesis and Characterization of Eco-friendly Alkaline Niobate-Based Composite Piezoceramics.
Supervisor: Prof. K. Chandramani Singh
Th 28459

Abstract

Piezoelectric ceramics are the functional materials which enable the interconversion of mechanical and electrical energy. For many decades, lead-based Pb(Zr,Ti)O3 (PZT) has been one of the most widely used piezoelectric materials in the electronic industry, due to its high Curie temperature and superior piezoelectric properties. However, lead-based electronic components phased out due to environmental concerns, safety concerns, and uncontrolled dispersion in the environment as the second most prioritized hazardous material by the EU. For more than two decades, researchers worldwide have sought lead-free piezoelectric replacements to toxic lead-based ones. KNN-based piezoceramics are considered a promising candidate among the different lead-free systems. This is due to their moderate piezoelectric properties, high Curie temperature (Tc), and low driving voltage, especially when the composition is close to the temperature-dependent phase transition known as polymorphic phase transitions (PPT). KNN-based piezoceramics are biocompatible and they can be used in a variety of sensors and actuators that are implanted directly into live organisms. In addition, they can readily be customized, which makes them an excellent option to lead-based PZT ceramics. Nevertheless, achieving well densified pure KNN ceramics using traditional sintering process is highly challenging due to the volatilization of alkali elements at higher temperatures. Due to inadequate densification, KNN-based piezoceramics experience significant problems during the poling process at high electric fields, resulting in a low piezoelectric value. We make an effort in the present study to further improve the characteristics of the KNN-based ceramics by synthesizing them via traditional sintering route through (a) investigating the impact of ABO3 component (Bi0.5Na0.5)ZrO3 on the electrical properties of (K0.485Na0.485Li0.03)(Nb0.96Sb0.04)O3 ceramic system, (b) Optimization of the preparation method for preparing KNN based ceramic systems and (c) studying the effect of dopants MnO2 and SnO2 on the piezoelectric properties and phase evolution of KNN based ceramic systems.

Contents

17. SAGAR (Puneet)

Fabrication of Piezoelectric ZnS-Based Flexible Nanogenerators and Enhancement in Their Output Performance via Chemical Composition Strategies for Energy Harvesting and Sensing.

Supervisor: Prof. Binay Kumar

Th 28741

Abstract

This thesis focuses on the development of flexible, efficient and low-cost nanogenerators for electrical energy harvesting utilising mechanical energy available in environment and wearable sensing applications as per the global need for sustainable energy alternatives. It explores piezoelectric, triboelectric and hybrid piezo-triboelectric nanogenerators (PENGs, TENGs and HPTENGs) as potential power sources for self-powered wearable/portable electronics and wearable sensing. The thesis describes the importance of ZnS as a possible piezoelectric material and the synthesis of ZnS, GO, PANI and biowaste-derived activated carbon nanostructures, and the fabrication process for flexible nanogenerators. It also describes the characterization tools used to study the structural, morphological, dielectric and

electrical properties of synthesized materials. Systematic studies were carried out to improve the output performance of ZnS-based PENG. Er-doped ZnS nanoplates and a modified electrode-based PENG showed significantly improved output performance. The Nd-doping further enhanced the voltage and power density of ZnS-based PENG, which was able to operate low-power electronics such as LEDs and wristwatches. GO-wrapping improved the polarization and dielectric behavior of ZnS nanoplates, which led to an enhanced piezoelectric output for efficient biomechanical energy harvesting and real-time human motion sensing. Then, to overcome the limitations of individual PENGs and TENGs, the Hybrid-PTENGs were developed. PANI-reinforcement in ZnS/PDMS composites showed enhancement in dielectric properties and delivered high electrical outputs suitable/enough for operating wearable/portable electronics. Finally, a sustainable approach was demonstrated to convert citrus-fruit waste into hierarchically porous activated carbon, which further enhanced the output performance of ZnS/PDMS-based HPTENG and enabled self-powered sensing for security applications. Overall, this thesis presents a comprehensive pathway from material design for the fabrication of flexible, eco-friendly and high-performance nanogenerators for next-generation self-powered wearable technologies. All the thesis work have been published in six peer reviewed international journals like JALCOM, MRB, AppNanoMat, AdvMatTech, etc. and presented in four conferences.

Contents

18. SAHDEV (Vandana)

Beyond the Standard Model Phenomenology with Exotic Fermions and Scalars.

Supervisors: Prof. Debajyoti Choudhury and Prof. Kirtiman Ghosh

Th 28742

Abstract

The Standard Model (SM) is an elegant theory that has stood many a tests. However, there are observations that compel us to look beyond the SM (BSM). The high energy colliders looking for BSM particles form an integral part of this quest. As part of this thesis, we explore the phenomenology of two BSM models that are primarily motivated from solutions to the issue of neutrino masses. In the first model, we investigate the potential of vector-like (VL) fermions in simultaneously addressing the issues of neutrino masses, dark matter and the discrepancies in anomalous magnetic moments of electron and muon. The light neutrino masses and mixings are generated radiatively while maintaining consistency with bounds on lepton flavor

violation. Loop diagrams with the very same fields also serve to explain the anomalous magnetic moments. Similarly, the correct dark matter relic abundance is reproduced without coming into conflict with direct detection constraints, or those from big bang nucleosynthesis or the cosmic microwave observations. Finally, prospective signatures at the Large Hadron Collider (LHC) are discussed. In the second model, we undertake the collider study of quintuplet fermions motivated from a model that generates neutrino masses via dimension-9 operator. We focus on the restricted model with quintuplet fermions and quartet scalars. In the standard scenarios, the exotic fermions decay directly to the SM particles and there exists a strong limit on their masses from collider experiments such as the LHC. We choose a particular scenario where the quintuplets are heavier than the quartets and show that it is possible to predict non-standard signatures at the colliders. We study these non-standard interactions and provide alternative search strategies for these exotic fermions at the LHC and the future linear colliders. We conclude the analysis by providing their exclusion and discovery limits.

Contents

1. Introduction 2. Massive neutrinos, anomalous magnetic moments and dark matter: Theoretical framework 3. Massive neutrinos, anomalous magnetic moments and dark matter: Results and collider prospects 4. Alternative signatures of the quintuplet fermions at the LHC and future linear colliders. Summary and Conclusion, Bibliography.

19. SAINI (Nidhi)

Physical Nature of Fast Radio Bursts and Some Observed Trends in Their Population.

Supervisors: Prof. Sourav Sur and Prof. Patrick Das Gupta

Th 28743

Abstract

Fast Radio Bursts (FRBs) are brief flashes of radio waves lasting milliseconds, likely caused by the gravitational collapse of rapidly spinning neutron stars. Our first work presents that the repeating burst FRB 121102A can be modeled within this framework. We suggest that the neutron star may implode into a Kerr black hole or transform into a strange quark star. n the case of Kerr BH formation, plasma winds from the observed near-by AGN impinging in the vicinity of the Kerr BH can lead to the emission of radio waves by virtue of the Blandford-Znajek mechanism. On the other hand, in the case of a strange quark star formation, the AGN wind perturbs the electron layer on the surface of the quark star, giving rise to radio emission in the GHz frequency range. We also introduce a common progenitor scenario for both FRBs and long gamma-ray bursts (GRBs) which in turn can lead to neutrino emission as well. The Canadian Hydrogen Intensity Mapping Experiment (CHIME) has detected numerous fast radio bursts (FRBs) and made the data publicly available. In our analysis of CHIME and non-CHIME sources, we find that FRBs can be categorized into two types based on peak luminosity densities. We propose that these FRBs may result from magnetar glitches, where sudden spin-ups of the compact star lead to abrupt changes in the light cylinder radius. The Hubble tension encapsulates a paradoxical discrepancy between two fundamentally different measured values of the Hubble parameter H0. In this ongoing work, how these differing values of H0 shape our understanding of distances, energetics, and the intricate properties of the FRBs is investigated. At last, we conclude with a summary and discussion of the outcomes of our research investigations.

Contents

20. SAO (Ajay Kumar)
Development of Sensing Layers for the Detection of Chemical Warfare Agents/Simulants.
Supervisor: Prof. Arijit Chowdhuri
Th 28460

Abstract

Abstract: Over the past century, chemical warfare agents (CWAs) have been extensively used as highly toxic synthetic compounds, resulting in severe harm or even death to humans. Nerve agents, despite being structurally similar to organophosphorus-based pesticides, are significantly more toxic to humans. One such lethal CWA is Sarin (RS-propan-2-yl methylphosphono fluoridate, GB), which belongs to the G-type organophosphorus compounds. Due to the extreme toxicity of Sarin and other CWAs scientists in laboratory settings utilize less harmful substitutes, known as simulants, to study the behaviour of CWAs. One such agent is DMMP (Dimethyl-methylphosphonate), due of its comparable structure and functional groups, DMMP has been researched as a Sarin mimic. Apart from the detection of the nerve agents and its simulants, detection of nitrogen dioxide (NO2) gas becomes very important because NO2 gas is used in the synthesis and disposal of the nerve agents and its simulants at precursor stage. The research work conducted for the thesis focuses on the development of bare SnO2, bare CdS and CdS-SnO2 thin film-based nanocomposite sensors, layered structure sensors and QCM sensors for the trace level detection of NO2 gas and DMMP vapours. SnO2, CdS and CdS nanocomposite have been synthesized using chemical route and the thin films of bare SnO2, bare CdS and CdS-SnO2 nanocomposites have been deposited onto IDE/glass substrate using spin coating technique. The fabricated sensors were utilized for NO2 gas sensing at 10 ppm concentration. Further the SnO2, CdS and CdS – SnO2 layered structure thin film have been grown using Rf – Sputtering technique. And the SnO2, CdS and CdS – SnO2 layered structure thin film-based sensors were utilized for NO2 gas and DMMP vapour sensing. Further CdS nanoparticle thin film base QCM sensor were fabricated using chemical solution deposition technique. And the fabricated sensor was employed for DMMM vapour sensing.

Contents

21. SINGH (Karsimran)
Study and Development of Supercapacitors having Gel Polymer Electrolytes and Biomass Derived Electrodes for Achieving High Energy Density Electrochemical Storage Devices.
Supervisor: Prof. Amarjeet Kaur
Th 28461

Abstract

The advancement of energy storage devices, particularly supercapacitors, is greatly enhanced by the development of advanced gel polymer electrolytes (GPEs) and the utilization of activated carbon materials derived from biomass sources. The work presented in this thesis systematically investigates the synthesis and performance of porous activated carbons obtained from biomass waste (citrus limetta pulp and sunflower seeds' shell (SSS)), employing both physical and chemical activation routes alongside various pretreatment strategies to optimize surface area and porosity. Additionally, the study presents the fabrication of various novel, different types of GPEs incorporating redox additives, ionic liquids, and plasticizers through the solution casting method, aiming to boost the energy density of supercapacitor cells. Structural characterization of the activated carbons was conducted using X-ray diffraction (XRD) and Raman spectroscopy, while morphological analyses using SEM and FESEM revealed the extensive porosity on the carbon surfaces. Surface area and porosity have been studied through the BET surface area analyzer and indicated a maximum surface area of approximately 1307.90 $m^2\ g^{-1}$ for SSAC (sunflower seeds' shells derived activated carbon), with HZAC (hydrothermal treated citrus pulp derived activated carbon) demonstrating the highest pore volume of around 0.88 $cm^3\ g^{-1}$. The optimized GPEs exhibited ionic conductivities in the order of 10^{-3} S cm^{-1} and demonstrated robust thermal stability, as confirmed by thermogravimetric analysis. The electrochemical potential window (ESW) of GPEs is found by using linear sweep voltammetry (LSV). The energy density of the cells varies with the type of GPEs used. Furthermore, modification in activation and pretreatment methods of biomass was found to substantially enhance the surface and electrochemical properties of the activated carbons, thereby improving ion transport and charge storage capabilities. Supercapacitor devices were fabricated using various combinations of activated carbons and GPEs, achieving a maximum specific capacitance of approximately 468.64 F g^{-1} in Cell-2 (having SSAC electrodes with HQ redox additive-based GPE), comparable to commercial grade and an energy density as high as 68.26 Wh kg^{-1} in Cell-10 (having HZAC cathode with EC/PC plasticizer-based GPE). These results highlight the critical role of material optimization and tailored electrolytes in advancing high-performance supercapacitor technologies.

Contents

1. Introduction 2. Methodology, Fabrication and Characterization Techniques 3. Structural and Morphological Analysis of Synthesised Different Activated Carbons 4. Redox Additive based aqueous Gel Polymer Electrolyte with Activated Carbons based Quasi-solid-state supercapacitors 5. Biomass-Derived Activated Carbon Electrodes in Quasi-Solid-state Supercapacitors Using Ionic Liquid Gel Polymer Electrolytes 6. Solid-State Zinc Ion Hybrid Supercapacitor based on Biomass Derived Activated Carbon and Plasticizer based GPE 7. Summary and Future Perspective.

22. SUMANA DEVI

Directional and Thermal Properties of Hindered Rotor in External Fields.

Supervisor: Prof. Vinod Prasad

Th 28462

Abstract

Hindered quantum rotors have been a subject of significant theoretical and experimental interest due to their unique properties under confinement. The

energy spectra, directional properties, and thermal behavior of hindered rotors exhibit substantial deviations from free rotors. These systems find applications across diverse fields, including molecular physics, nanotechnology, and material science, due to their relevance in areas such as molecular alignment, rotational spectroscopy, and quantum information processing. With advancements in experimental techniques, there is an increasing demand for a detailed theoretical understanding of hindered rotors under various confining potentials. The present study focuses on analyzing the impact of hindering potentials, including external fields and confinement strength, on the directional and thermal properties of hin dered rotors. Special emphasis is given to the study of the hindering potentials for a single rotor in external electric fields, however, we also analyse the rotational dynamics of a coupled pair of hindered rotor in external fields, which are relevant for understanding the behaviour of many quantum molecular systems and related applications. Analytical solutions to the Schrödinger equation for hindered systems are limited to the lowest few energy states; however, numerical approaches allow the determination of energy eigen values and other properties for a much larger number of states. In this work, hindered rotor systems that we have studied are: a single rotor confined in a well-shaped confinement, a diatomic molecule adsorbed on a surface, and a coupled pair of hindered rotor. We solve the non-relativistic Schrödinger equation numerically for these modelled systems in external fields to get energy eigenvalues and eigenvectors. Then we explore the rotational dynamics, directional and thermal properties of these hin dered rotor systems by exploiting the rotational energy spectra. The dependence of orientation and alignment parameters on static electric field and confining potential is studied. We compute thermal properties like entropy and heat capacity of the system under consider ation using the canonical partition function within statistical thermodynamic formalism. We have also studied the effect of external field parameters, confinement strength, and tem perature on these thermal properties. We also investigate how laser frequency, amplitude, and hindrance strength influence transition probabilities. The combined effect of coupling and external fields on the energy spectra, directional, and thermal properties of the coupled hindered rotors is also explored.

Contents

23. TAMTA (Suraj)
Metal Embedded Silica Nanostructures: Plasmonic Aspects and Applications.
Supervisor: Prof. P. Senthil Kumar
<u>Th 28464</u>

Abstract

Silicon dioxide (SiO2), the most common semiconducting substance, is found in numerous rocks, minerals, and valuable and semiprecious stones. Stöber et al. stabilized the synthesis technique for silica particle shape/size distribution, which Van Heldenet al. investigated further using scattering and microscopy. Xia et al proposed that PVP has a modest reducing capacity due to the presence of hydroxyl (-OH) groups in the reduction of Ag+ ions. A strong hydrogen connection exists between the carboxyl group in PVP and for the durability of the coating, refluxed silica in PVP aqueous solution at a certain concentration of SiO2/PVP is used. While reviewing the reduction ability of PVP for metal nanoparticles, the core-shell structure became a subject of interest, which provides an enhancement in physiochemical properties and stability against nanoparticle aggregation. The galvanic replacement process is well known in aqueous solution, but it differs on a dielectric surface from a solution in which Ag nanoparticles provide a symmetric contact for all Au atoms. Because of the attachment of Ag nanoparticles to silica, the surface`s active area for Au is limited, resulting in an Au shell around the silica spheres that exhibits mixed spectra for both Ag and Au nanoparticles on silica depending on the percentage of Ag (inner) or Au (outer) nanoparticles. Our combined data analysis (using XRD, FTIR, and UV-Vis spectroscopy measurements) confirms the plausible mechanism governing substrate-based galvanic replacement reactions using PVP functionalized silica spheres, establishing only the careful and robust formation of Ag@Au core-shell onto silica spheres rather than their hollow counterparts. Furthermore, we created the corresponding monolayer films using the well-known air-water interface self-assembly process, allowing us to easily adorn various surfaces with a uniform array of these surface-coupled metal nanoparticles. Enhanced sensing applications.

Contents

24. YADAV (Chanchal)

Structural Properties of Confined Atomic Systems and Their Response to External Fields.

Supervisors: Prof. Vinod Prasad and Prof. Poonam Silotia

<u>Th 28465</u>

Abstract

Quantum confined systems have been a topic of vast exploration in theory and experiments. The system's properties, like energy spectrum, ionization energy, excitation energy, oscillator strength, polarizability etc., change greatly compared to free systems. Quantum confined systems are useful in various applications, such as semiconductor technology, optoelectronics, and medical science. With advances in experimental techniques, it is crucial to understand these systems theoretically. The interaction potentials of constituent charged particles of embedded atom are modified by plasma screening. Various factors like size of boundary, and shape of potential are key parameters used to study the properties of confined particles. This work focuses on comparative study of spherically confined hydrogen atom under different modified ring-shaped potentials. Due to non-existence of analytic solutions of Schrodinger equation for such confined system, we have solved numerically using 9-point FDM. We have established accuracy of our results by comparing them with known theoretical results for free system. The electronic structural properties of an atom embedded in finite-density plasma at a specific temperature are well known to differ from free-state atom. The mean distance between particles reduces as plasma density increases, resulting in inter-particle contact and non-ideality of plasma. To understand effect of non-ideality of plasma potential, comparison of structural properties of confined hydrogen atom embedded in non-ideal classical potential is obtained. Dipole-dipole interaction is an anisotropic, non-central interaction potential. Due to small transient dipole moment of hydrogen atom, it is interesting to

study a system of two hydrogen atoms interacting via this potential. We have formulated collision dynamics of a pair of hydrogen atoms under external static electric field via dipole-dipole interaction. Towards, the end of this work we have explored behaviour of spherically confined hydrogenic systems under Poschl-Teller double-ring-shaped Coulomb potential. The possibility to induce persistent currents within the s-states is explored.

Contents

25. YADAV (Tarun)

Performance Enhancement of KNN-Based Lead-Free Piezoelectric Perovskite Materials for Energy Harvesting Applications via Doping, Phase Boundary Engineering and Shock Treatment.

Supervisor: Prof. Binay Kumar

Th 28466

Abstract

The thesis presents the development and optimization of lead-free piezoelectric ceramics as environmentally friendly alternatives to conventional lead-based materials such as PZT. Driven by the growing demand for sustainable, high-performance materials in sensors, actuators, and energy harvesting systems, this work focuses on potassium sodium niobate (KNN)-based ceramics due to their promising piezoelectric and thermal characteristics. A multi-faceted strategy combining internal structural modification and external treatment was employed to improve key material properties. The first approach involved vanadium doping in $Na_{0.46}K_{0.46}Li_{0.08}NbO_3$ (NKLN) ceramics. This substitution enhanced remnant polarization, improved piezoelectric charge coefficient, increased mechanical hardness, and improved the energy harvesting response when embedded in a flexible PDMS matrix and deposited on ITO/PET substrates. Building on this, a second strategy employed phase boundary engineering by incorporating $Bi_{0.5}Na_{0.5}TiO_3$ (BNT) and $Bi_{0.5}K_{0.5}ZrO_3$ (BKZ) into the KNN matrix to establish a rhombohedral–tetragonal phase boundary. This resulted in a high piezoelectric charge coefficient (d_{33} = 407 pC/N), stable dielectric behavior, and improved reliability over long-term electrical cycling. To further enhance performance, shock wave treatment was applied to KNN ceramics co-doped with BNKT and $BiGaO_3$. Post-shock treatment analysis revealed microstructural refinement, increased Curie temperature, and improved piezoelectric output. The treated ceramics were integrated into flexible microgenerators, which exhibited open-circuit voltages up to 38 V under mechanical and shock excitations. The research culminated in the synthesis of a novel NKLNS-BS-BNTZ composite engineered at a morphotropic phase boundary (R–O–T), which demonstrated excellent piezoelectric performance (d_{33} = 375 pC/N), acoustic energy harvesting capability, and resilience under harsh conditions. Collectively, the study highlights the synergistic impact of doping, phase design, and external stimuli in tuning the performance of lead-free piezoceramics, offering scalable, application-ready materials for next-generation flexible electronics, aerospace, and energy harvesting technologies.

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