CHAPTER 42

PHYSICS AND ASTROPHYSICS

Doctoral Theses

01. ANJU
Phenomenological Study in Heavy Ion Collision.
Supervisor: Prof. S. Somorendro Singh
Th 26839

Abstract

The theory of strong interaction describes quantum chromo dynamics. The dynamics of quarks and gluons can be understood theoretically with the help of QCD. The striking features of QCD are the spontaneous breaking of chiral symmetry and confinement. The interaction among quarks gets weaker when distance between them decreases and this feature is known as asymptotic freedom. However the interaction between them becomes stronger as the particle separation increases. A quantitative understanding of this phenomena called confinement is hard to obtain even though we know the underling theory. Due to the non abelian nature of QCD it is very hard to understand the interaction between quarks and gluons as the inclusion of gluon self interaction terms. Thereby it is very difficult to solve the QCD equations on a purely mathematical ground. The alternative way to solve such problems using perturbation theory at short distances is considered in a strong coupling regime relevant to nuclear physics. Another way to solve such a problem is trough the numerical calculations of QCD on a discrete four dimensional space time lattice. With this understanding our aim is to study QCD using PNJL model by understating different thermodynamic properties of a system and further investigate how PNJL model gets affected by the action of magnetic field and temperature dependent quark mass. We will extend this study by introducing a magnetic field and temperature dependent quark mass for 2 and 2+1 flavor quarks.

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02. ASAR AHMED
Development of GEM detectors for the CMS Experiment and its Application to Imaging, and Vector Boson Scattering Measurements at LHC Energies.
Supervisor: Prof. Mohammad Naimuddin
Th 27173

Abstract

The standard model framework of particle physics describes a basic architecture for electromagnetic strong and weak interactions. Despite its enormous successful implications the model has various limitations as it does not answer satisfactorily questions like matter antimatter asymmetry hierarchy problem nature of dark matter etc. One of the vital questions how elementary particles gain their masses is explained in the SM via the brout englert higgs mechanism. According to the BEH mechanism all massive particles acquire their mass through interaction with the higgs field. A similar particlewith a mass of 125 GeV and feadturing properties as that of the SM higgs boson was reported by the ATLAS and CMS collaborations in 2012 at CERN. The electroweak symmetry is spontaneously broken in the standard model when a scalar field. Higgs is introduced. This field generates four degrees of freedom one of which is the higge boson and the other three constitute the longitudinal modes of the weak bosons W+, W- and Zo. From the theory the symmetry breaking sector may be directly investigated by the scattering of heavy electroweak bosons. Higgs boson itself plays an important contribution in regularisation of the scattering amplitude which in the absence of the higgs boson violates unitarily at high energies. The characteristics of the higgs boson that are not consistent with the SM may also be seen through vector boson scattering and can be a power tool to test effects beyond SM. The VBS events are purely electroweak and has a lot of background con-tamination at LHC which makes is rare [rpcess. Due to the enough data collected by the LHC experiments in recent years it is now feasible to exploit this sector. The current work is carried to explore VBS processes through semileptonic channel. The analysis is performed on the data accumulated by the CMS during the years 2016 to 2018 at 13 TeV of energy corresponding to an integrated luminosity f 1338 fb-1. The thesis presents the very first evidence for the EW production of a WV (V=W or Z) pari plus two jets in semileptonic decay channel where W decays leptonically and V decays hadronically. The event categorization technique is exercised to enhance sensitivity and the one appearing in the highest expected significance has been preferred.

Contents

03. BALA (Nisha)
Microstructural and Raman Spectroscopic Investigations of the Magnetic Ordering in NiO Nanoparticles.
Supervisor: Prof. Shyama Rath
Th 27178

Abstract

A transition from an antiferromagnetic behaviour in the bulk to a ferromagnetic one when the size is reduced to nanometric NiO is an interesting material for both ferromagnetic and antiferromagnetic spintronics. The goal of this work is to understand the size and stoichiometry dependnt magnetic ordering of nanocrystalline NiO using raman spectroscopy. The synthesis method has a significant influence in controlling the size quality reproducibility and size dependent properties of NiO nanoparticles. NiO nanoparticles used for the study

are prepared by sol gel technique commercial NiO nanopowders and prepared by hydrothermal technique. The effect of the annealing atmosphere and temperature on the microstructural and magnetic properties of sol-gel synthesized NiO nanoparticles are investigated. A structural refinement of the X-Ray diffraction pattern shows an increase in particle size with a decrease in lattice constant and bond length with increasing annealing temperature. Air annealing leads to larger variation in sizes as compared to oxygen annealing. For moderate oxygen annealing up to 600o C a Ni phase is observed which is almost undetectable for air annealing. The size dependent structural properties are further analysed by transmission electron microscopy. The colour is a good indicator of non-stoichiometry and shows clear changes with the annealing conditions as determined from energy dispersive X-ray spectroscopy. Magnetic properties are extracted from the law of approach to salutation fit of the magnetic hysteresis curves.

Contents

04. BHUSHAN (Ravi)
Search for Exotic Nuclear Shapes at High Spins in Nuclei of Mass A-150-190.
Supervisor: Prof. S.K. Chamoli
Th 26849

Abstract

In the present thesis work, we report the nuclear shape properties at high spins in 187Hg, 177Re, and 151Dy using the lifetime measurement technique. The experiments were done with energetic high beams delivered by the 15UD (16-MV) Pelletron Accelerator facility available at the Inter-University Accelerator Center (IUAC), Delhi. For detection purposes of gamma rays, the Gamma Detector Array (GDA) setup and Indian National Gamma Array (INGA), available at the Inter-University Accelerator Center (IUAC), Delhi were used. All level lifetimes were measured by the Recoil Distance Doppler shift Method (RDM) using a plunger setup. For production of high spin states in 187Hg, 177Re and 151Dy following nuclear reactions were used. • 159Tb (32S, p3n) 187Hg @ Elab = 154 MeV • 165Ho (16O, 4n)177Re @ Elab = 84 MeV • 128Te (28Si, 5n) 151Dy @ Elab = 145 MeV The experimental B(E2) and Qt values extracted from the measured level lifetimes were compared with the results of the TRS calculations, done within the framework of Cranked Hartree-Fock Bogoliubov (CHFB) model and the results of the projected shell model (PSM) calculations. The 187Hg nuclei lie toward the upper end of A ∼ 150 - 190 mass region. This region is better known as a region of shape coexistence. In this mass region apart from Hg isotopes, the evidences of shape coexistence are being reported in the neighboring Pb, and Pt nuclei too. The available data suggest that in even-even Hg nuclei of this mass region, shape mixing xx Abstract rather than shape coexistence is more prevalent. The odd–A Hg nuclei of this mass region, on the other hand, seem to behave a little differently than their even-even neighbors. The observed rotational bands, one based on the K π = 9/2 + orbital from the i13/2 neutron shell at low excitations and the other based on 13/2 + isomeric state at little higher excitations, in general support the shape coexistence picture in 187Hg. Also, as observed in the neighboring even-even Hg nuclei of this mass region that a substantial mixing takes place at various spin values of the

yrast states, there is a fair chance that the yrast states in 187Hg nucleus are mixed too. By comparing the experimentally measured B(E2) values for different gamma transitions along the yrast band with the results of the band mixing model calculations, a reasonable estimate of the mixing (if any) of the two coexisting bands can be obtained in 187Hg nucleus. The Re nuclei fall near the middle part of this mass region (A ∼ 170) between the strongly deformed rare-earth nuclei and the spherical lead isotopes. This region is considered as transitional region. For Re isotopes, the nuclear structure is highly configuration dependent. The proton Fermi surface lie near to the highly downsloping low Ω, high-j orbital like πh9/2 and πi13/2 orbitals intruding from above the Z = 82 shell closure so deformation driving tendency of orbitals is expected in Re nuclei. In fact previous lifetime measurement study in 177Re, the deformation of intruder low Ω high-j orbitals πh9/2 is found to be ∼ 23 % and ∼ 15 % higher than the upslopping proton orbitals like πd5/2 and πh11/2 respectively. Also the B(E2) values show gradual increment for high-K πd5/2 (α = −1/2) (Band 2), which has been is interpreted as β-stretching characteristics of this band. On the other hand, the nearly constant behavior of B(E2) values with increasing spin in πi13/2 (Band 3) give an indication of the stable nuclear configuration. In the present work, the observed high Qt values of πi13/2 band also indicate the larger deformation (∼ 27 % more) as compared to πd5/2 (α = −1/2) (Band 2) in this nucleus. It means if an odd proton occupied the πi13/2 orbital have a strong polarizing effect on the even-even core and drives the nucleus toward more deformation. The Dy nuclei fall in the lower edge (A ∼ 150) of this mass region have rich structural properties. The valence protons and neutrons in these Dy nuclei occupy high spin orbitals like πh11/2 (by protons) and ν f7/2 , νh9/2 , and νi13/2 (for neutrons) and therefore carry xxi high angular momentum. The low spin spectra in odd-A Dy nuclei of this mass region (e.g. 149,151,153Dy) is characterized by single particle states formed by the valence nucleons by aligning their angular momentum. As these excited states are fed from the top so depending upon the pattern of feeding states, 'yrast isomers' and 'yrast traps' are also very much expected in these odd-A Dy nuclei. The 151Dy has two valence protons and three valence neutrons compare to even-even 146Gd core. This nucleus is predicted to be oblate deformed in its ground state. The occurrence of irregular energy spacing between the energy levels and the presence of nanosecond (ns) isomers in a way indicate the oblate deformation of 151Dy. In fact, in the previous experimental studies, the observed long-lived isomer (τ = 10.9 ns) at J = 49 2 in 151Dy also support the oblate deformation, However, there are other high-spin isomers which are observed in 151Dy some of which are not seen in other members of N=85 isotones. This puts an overall again question mark on the configuration of those isomers and the overall deformation of nucleus and therefore makes deformation studies in 151Dy absolutely necessary. The irregular nature of B(M1) values observed in our measurement do indicate the non-collective states built on the oblate deformed core in 151Dy. So, the 187Hg, 177Re, and 151Dy nuclei reported in this work, in general, exhibit the nuclear structure properties of their mass region quite well. The present data, however, seem to be insufficient to resolve all issues observed at high spins in all nuclei, and therefore further measurements are required. Especially in 187Hg, where present studies indicate a sudden change for oblate to prolate shape afterward 21/2+ spin along the yrast band, to settle the nature of deformation (prolate or oblate) of the yrast band, further measurements like Coulomb excitations are needed in 187Hg nucleus

Contents

05. BHARATI (Manisha)
Fobrication of Lamb Wave Based Acoustic Devices for Realization of Sensing Platform.
Supervisor: Prof. Monika Tomar
Th 26840

Abstract

In the present era of industrialization, the sensors not only ease up individual's life style but also improve the societal standards through environmental monitoring, medical diagnostics, improved safety and security, enhanced performance of energy sources such as solar power and fuel cells, besides exploration in aerospace technology. In the present world, the sensors have been so assimilated in our life that many a times we do not even notice their presence. Quest of researchers and engineers for sensors has induced development of several types of sensors. Among those, the acoustic wave based sensors have advantages of stable fundamental frequency, high sensitivity, room temperature operation, compact size, portability, long shelf life along with the possibility of wireless integration. The acoustic wave based sensors have a disadvantage of complicated fabrication steps. However, the tremendous potential of these sensors, to be employed in remote and harsh environmental conditions with high sensitivity, good stability and good reproducibility, outweigh the disadvantage and encouraged the present work to focus on the acoustic wave based sensors. Acoustic wave is classified as Bulk Acoustic Wave (BAW) and Surface Acoustic Wave (SAW). Both types of the waves are used for sensing applications. Further, among various types of SAW devices, the Lamb wave based devices have highest mass sensitivity since the entire device is fabricated on a membrane, it makes this device favorable to use in sensing applications. Moreover, the Lamb wave resonator may provide a good alternative because it combines the advantages of SAW devices and thin film based BAW resonators. Therefore, in the present work, Lamb wave based sensors have been utilized for various sensing applications. Lamb wave is a type of surface acoustic wave with saggital wave propagation where the substrate thickness is lesser than the acoustic wavelength. The Lamb waves are unique in their characteristics in existence of two modes, namely antisymmetric and symmetric modes. Besides the fundamental mode of the Lamb wave device, its higher modes can also be used for sensing applications. Having advantage of higher velocity of wave propagation, higher mode shows higher relative velocity shift in the presence of any analyte, leading to higher sensitivity of the device. vii In order to explore the vast potential of the Lamb wave device for sensing applications, the present work aims toward optimization and fabrication of Lamb wave based devices using piezoelectric ZnO thin film on SiO2/Si membrane. For theoretical studies, finite element analysis followed by modelling and simulation techniques involved in COMSOL multiphysics software have been discussed. Optimization of several layers of Lamb wave device have been discussed for attaining the high acoustic velocity with good electromechanical coupling coefficient. As higher frequency attributes toward higher sensitivity of the Lamb wave device, simulations have also been performed to study the higher frequency modes of the ZnO/SiO2/Si membrane based Lamb wave devices. For the fabrication of Lamb wave device growth and characterization of the piezoelectric ZnO thin film over SiO2/Si membrane and performance study of the finally fabricated devices have been discussed. The experimentally obtained results are also compared with theoretically obtained values. The fabricated Lamb wave devices have been explored for biosensing, physical sensing and chemical sensing applications. For the biosensing application of Lamb wave device, DNA of

bacterial meningitidis has been chosen. For the realization of Lamb wave as a biosensor, biosensing layer of ZnO thin film has been grown inside the cavity of the Lamb wave device. The probe (single stranded DNA oligomers) have been immobilized inside the cavity using physical adsorption technique. The binding of complementary DNA strand present in the test sample, over the immobilized probe DNA confirms the presence of bacterial meningitidis. The indigenously developed biosensor shows a very high sensitivity of 310 Hz(ngµl-1) -1 and very low detection limit of 82 pgµl−1 for fundamental symmetric mode of the Lamb wave device while the fundamental antisymmetric mode shows a sensitivity of 202 Hz(ngµl-1) -1 and the limit of detection of 84 pgµl−1 . Further for sensing physical analytes, UV rays and pressure (≤ 1 atm) were selected. For UV detection, ZnO thin film grown on SiO2/Si membrane has been used as the sensing layer. Electrical studies of the fabricated ZnO/SiO2/Si Lamb wave resonator device reveal a change in current (ION/IOFF ~ 104) upon UV illumination (λ = 365 nm, Intensity = 0.2 mW/cm2) with a high value of responsivity (46.95 A/W) and detectivity (5.4×1012 Jones). The response and recovery time was observed to be 280 ms and 25 ms respectively. It is observed that the highest mode (A2) of Lamb wave resonator (192.27 viii MHz) shows maximum sensitivity towards UV radiation resulting in a frequency shift of 535 kHz(mW/cm2) -1 and very high sensitivity of 2.78 × 103 ppm(mW/cm2) -1 . In addition, various mechanisms involved in the photodetection are discussed. The effect of induced piezo-potential on Schottky barrier height in the acoustic device and corresponding enhancement in the photodetector performance are discussed along with the experimental studies. For pressure sensing application, a pressure range less than the atmospheric pressure is chosen. Based on the confinement of bulk wave in the acoustically rarer silicon medium, higher overtone of bulk acoustic resonance in ZnO/SiO2/Si membrane is obtained. For a pressure range of 49 kPa to 100 kPa, the fabricated sensor has shown a pressure coefficient of frequency (PCF) value of 13.66 ppm/kPa at room temperature, while for a pressure range below 0.7 kPa the PCF value is observed to be 1382 ppm/kPa. For chemical sensing application of Lamb wave device, two different chemical warfare agent (CWA) simulants were chosen: (a) Dimethyl methylphophonate (DMMP) and (b) Dibutyle Sulphide (DBS). Multiple sensing layers, including SnO2, TiO2 and ZnO were grown on the ZnO/SiO2/Si Lamb wave device and all were deployed for sensing of both DMMP and DBS. It was observed that for the DMMP sensing, SnO2 based Lamb wave device has shown maximum sensitivity with a value of 4.25 kHz/ppm. While for DBS sensing, among SnO2, TiO2 and ZnO sensing layers, the ZnO sensing layer based sensor showed maximum sensitivity of 2.98 kHz/ppm. Finally all the CWA sensing devices were studied in terms of polar plots to detect the presence of distinct CWA in terms of different patterns for each type of CWAs.

Contents

06. BHARTIYA (Prashant Kumar)
Designing and Development of Chiral Magnetic Electrodes for Efficient Spin-Based Water Splitting.
Supervisor: Dr. Debabrata Mishra
Th 26841

Abstract

Dissociating water molecules to generate hydrogen gas decreases dependence on hydrocarbon-based energy sources. Water splitting/dissociation involves both oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). Smart electrodes are needed for efficient water splitting to provide sustainable hydrogen energy. In addition to the geometrical optimization of participating electrodes, the spin of electrons is critical during the oxygen evolution process. It is generally known that during water splitting, the synthesis of the O2 molecule happens in a spin triplet state, preventing the production of the spin singlet state of H2O2. The focus of the thesis work is to develop such electrodes that can produce spin-polarized electrons to enhance OER. One of the ways to achieve spin-polarized electrons on the surface of the electrodes is to functionalize the electrode with chiral molecules which behave as spin filters to yield spin-polarized electrons. Chiral molecules generate spin-polarized electrons due to the inversion asymmetry present in their primary or secondary structure and this phenomenon is known as chiral induced spin selectivity (CISS) effect. To accomplish this, magnetic electrodes such as Ni/Au and Ni/Al have been prepared and functionalized with chiral molecules including L-Cysteine, DPhenylalanine etc. to generate spin-polarized electrons. Subsequently, the catalytic properties of these chiral electrodes have been tested for overall water splitting, including OER and HER. The effect of substrate, light and magnetic field on the spinbased water splitting has been investigated on reduced graphene oxide and its composites on nickel foam. The impact of chirality on overall water splitting relative to primary structure is examined in depth for biomolecules with secondary structures like the DNA helix. It has been concluded that electrons' spin plays an important role in enhancing OER activity significantly and improves overall water splitting.

Contents

07. DAS (Jaydeb)
Rare Semileptonic Decays of the Ab in the Standard Model and Beyond.
Supervisors: Prof. Debajyoti Choudhury and Dr. Diganta Das
Th27259

Abstract

The flavour changing neutral current transition b-→sl+l- being both loop and CKM suppressed in the SM offers a promising ground to search for tiny effects of NP. In the past decade a series of experiments testing LFU violation in such transitions, had initially indicated a very significant significant deviation only to recently settle at marginal consistency. However further investigations of NP are warranted by the longstanding discrepancies in the differential branching ratios and the angular observables of b--→sl+l-. It should be remembered though that unlike canonical LFU observables (namely, overall rate comparisons) differential branching rations and angular observables are plagued by harmonic as well as other theoretical uncertainties. In chapter 2, we have studied some aspects of the Ab-→A*(-→NK)l=l- decay. The underlying b--→sl+l- effective Hamiltonian is extended by including the chirality flipped counterparts of the SM operators, and scalar and pseudo scalar operators. We have presented a full angular analysis where are have also retained the masses of the final state leptons. The angular observables are expressed in terms of the transversely amplitudes. The four-fold distribution allows us to construct several observables that we study in the SM and in model independent NP.

Contents

08. DARSHAN KUMAR

Estimation of Cosmological and Galaxy Parameters Using Statistical Methods.

Supervisors: Prof. Deepak Jain and Prof. Shobhit Mahajan

Th 27260

Abstract

In the last few decades the study of cosmology has moved into an era of pre-cise research. Using advanced measurement techniques and very sensitive instruments cosmological observations have given us a new understanding of the universe which was not possible before. In order to take advantage of more accurate observations of the universe it is necessary to use sophisticated statistical methods. In response to this challenge the field of data analysis has also changed a lot and there have been several innovations in the last few years in analysis of observational datasets. In this thesis we focus on using multiple observations and statistical techniques to estimate various cosmological parameters as well as galaxy parameters. The spatial cosmic curvature parameter Ω 40 is an important cosmological parameter which plays a crucial part in determining the dynamics of the universe. Its value can vary between 1 and +1 theoretically. Another key relation in cosmology in the cosmic distance duality relation which is specified by the parameter π. It is a relation between the luminosity distance of an object its redshift and its angular diameter distance. It should hold in any metric theory of gravity in which light propagates along null geodesics as long as the photon number remains conserved. Any deviation from this relation can potentially signal some new physics. Further we discuss the transition redshift which signifies a shift from a period of decelerated expansion

to one of accelerated expansion. We probe these parameters using both model dependent and model independent methods with recent and updated observational datasets.

Contents

1. Introduction. 2. Cosmology overview. 3. Cosmological observations and their implications. 4. Statistical techniques for data analysis in cosmology. 5. Cosmology with strong gravitational lensing systems. 6. Test of variability of type la supernovae luminosity. 7. Transition redshift using hubble phase space portrait. 8. Conclusions and future directions. References.

09. DAHIYA (Annu)
Plasmonic Simulation of Alloy, Dimer and Surface Oxidized Metal Nanoparticles.
Supervisors: Dr. Pandian Senthil Kumar
Th 26842

Abstract

Optical properties of metal nanoparticles (of dimensions significantly smaller than the wavelength of light) were first scientifically explained by classical electromagnetic (EM) theory. Their unusually vibrant colors were rightly attributed to the resonant collective oscillations of the conduction electrons with respect to the incident light, aptly termed as ‘surface plasmons,' that exist primarily in the visible/optical wavelength region for noble metals and in UV region for aluminum. In terms of managing the surface plasmon resonance in the required optical range, noble metal alloy nanoparticles easily achieve the potentials needed for specified applications. Additionally, the physical mixture emphasizing the inter-particle coupling between the nanoparticles themselves as well as external analytes offer a wide range of possibilities for manipulating the nanoparticle properties. Though such interactions between complex geometry nanoparticles are well-known for their diverse application capabilities, a fundamental understanding of the interaction between nanoparticles remain very limited, majorly due to their stability even under normal conditions. In contrast, the oxidation of metal nanoparticles itself can be utilized as an asset, for understanding its assorted application potentials. Subsequently, alloying, coupling and oxidation in metal nanoparticles along with their respective plasmonic signature are responsible for concentrating light on the nanometer scale in terms of their optical near-field, as explained by Maxwell's equation of EM waves. Novel methodologies based on theoretical approaches are readily available to explore the interaction of EM radiation with metal nanoparticles. In this thesis work, we have used BEM, in MATLAB based toolbox MNPBEM for in-depth analyses of such interactions utilizing plane waves, dipole emitters and electron beam, all of which highlights the important antenna-based applications. In summary, the light-matter interaction aspects of metal nanoparticles were analyzed in this thesis along with contrasting the simulated and experimental results, wherever applicable

Contents

1. Introduction. 2. Materials and methods. 3. Unveiling the plasmonic character of AuCu alloy nanoflowers and their applications. 4. Dipole emitter interaction-based antenna character of Ag and Au homodimer. 5. Spatial tunable plasmonic

nanoantenna character of Ag-Au heterodimer. 6. Site-selective oxidation modulated plasmonic resonances in AI nanostructures using electron-energy loss spectroscopy. 7.Summary and future prospects. Publications.

10. DEKA (Kuldeep)
Exploring Physics Beyond the Standard Model Through Effective Interactions.
Supervisors: Prof. Choudhury Debajyoti and Mandal Tanumoy
Th 26843

Abstract

In the thesis “Exploring Physics Beyond the Standard Model through E↵ective Interactions, we utilise higher-dimensional e↵ective interactions to probe various shortcomings of the Standard Model (SM) of particle physics, explore novel signatures for Beyond Standard Model (BSM) physics, and fit various BSM parameters to the experimental data. We begin our journey in Chapter 1 by briefly reviewing the SM along with its successes and shortcomings and presenting arguments in favour of implementing higher-dimensional e↵ective interactions. In Chapter 2, we work out a model building exercise by extending the SM gauge group with an extra U(1) and the particle spectrum augmented by three right-handed neutrinos (RHN) and two scalars. The gauge charges dictated by the anomaly cancellation conditions are assigned in such a way that dimension-4 operators are precluded in the neutrino sector and only higher-dimensional e↵ective operators can be written, which is then utilised in Chapter 3 to solve the problem of neutrino mass without resorting to any unnatural parameter choices. Heavy Z0 phenomenology gets altered because of the presence of the RHNs, which is also studied in detail in Chapter 3. We also show the viability of solving the problem of Dark Matter (DM) through this model. In Chapter 4, we study the prospects of obtaining TeV scale resonant leptogenesis in the same model discussed in Chapter 2 and also the models collider prospects. In order to get a comprehensive idea about collider analysis, in Chapter 5, we discuss a pure collider physics problem where we look at the prospects of a vector-like B quark at the LHC. We utilise a (dimension-5) chromomagnetic coupling in order to produce these heavy B quarks and study the discovery significance for this coupling by implementing jet-structure techniques in the fully hadronic final states. In Chapter 6, we undertake a comprehensive global fitting exercise. We first utilise dimension-6 SMEFT operators, where the SM is augmented with all possible non-redundant dimension-6 operators allowed by the SM gauge group, and fit their Wilson coe s and present the results of the fit. Finally, we summarise in Chapter 7.

Contents

11. GURJAR(Mukesh Chand)
Laser-Plasma Based Terahertz Radiation Generation.
Supervisor: Prof. D.N. Gupta
Th 26844

Abstract

The generation of terahertz (THz) radiation has been of significant field of research in last few decades due to its wide application range in various areas. Albeit, most of the THz mechanisms are not efficient enough to generate high-field THz due to their lower damage limit. To overcome this limitation, plasma is utilized as a nonlinear medium in various schemes employing a strong laser-plasma interaction. The motivation of this thesis is to explore various ways to generate THz fields using laser-plasma system. We have investigated a mechanism for high-field THz radiation generation by beating two chirped Gaussian laser beams in non-uniform plasmas. The mechanism is based on the strong transverse current generation in plasma via beating of two lasers. The resulting THz radiation is characterized by a transverse current and a broad spectrum with frequency is occurred near the beat-wave plasma frequency. The role of plasma channel has also been studied for better THz conversion efficiency. The plasma channel offers an extended guiding of the laser pulse, which further enhances the THz conversion efficiency. This work has been extended for electron-hole plasmas. In this study, we presented phase-matched terahertz radiation generation from laser interaction with electron-hole plasmas. A method for THz field generation without any phase-matching requirement has been explored in this thesis. A rotating electron beam has been used to excite plasma wakefields. The plasma wakefield couples with the electron beam to excite transverse currents at THz frequency. The THz field amplitude is controllable by the electron beam velocity and density. Such a compact source of THz radiation is not only triggering various nonlinear dynamics in matter, but also opens up the research era of relativistic THz optics.

Contents

12. HOR (Abbas Ali)
High Performance Carbon Supercapacitors Based on Lonic Liquid Incorporated Redox-Active Gel Polymer Electrolytes.
Supervisors: Prof. S.A. Hashmi
Th 26845

Abstract

Continuous use of fossil fuels like petroleum, natural gas, and coal has caused different environmental issues such as greenhouse gas emissions which affect human health, contribute to global warming. Fossil fuels are depleted over a short period of time, because of increase in the worldwide population and high demand of energy. Therefore, the researchers have shifted to a renewable source of energy, such as solar energy, wind energy, and industrial waste heat energy, which are environment friendly (produce energy without CO2 emission). However, most of these renewable energy sources are

intermittent or periodic in nature. As a result, energy storage devices are necessary for the efficient storage of energy released from these renewable sources. This growing requirement has encouraged the development of several electrochemical energy storage technologies, including fuel cells, batteries and supercapacitors. However, the need for high-performance energy storage systems is increasing because of the quick expansion of market for portable electronic gadgets. In order to meet the demands of both contemporary life and the needs of rising ecological concerns, new environmentfriendly and cost-effective energy storage systems are fundamentally needed. Supercapacitors, in addition to batteries and fuel cells, have drawn a lot of interest because of their favorable characteristics which includes high power density and long cycling life as compared to batteries, and significantly higher energy density in comparison to conventional and electrolytic capacitors. The above mentioned properties of the supercapacitor makes it suitable for various applications namely; memory protection, electric or hybrid electric vehicle (where supercapacitors delivers high power for the acceleration of the vehicle and get it charged during braking), backup in power electronics, battery enhancement (where supercapacitors protect batteries from high load demands by meeting the peak power requirements and permitting the batteries to provide average load), military and aerospace applications. In electrochemical energy storage devices like supercapacitors, batteries etc., electrolytes play a vital role in transporting ions from electrolyte to electrode surface or from one electrode to another. The characteristics of the electrolytes have a direct impact on the electrochemical performance of the energy-storage device. In order to vii qualify as an ideal electrolyte material, a substance must have the following properties such as: high ionic conductivity, wide electrochemical stability window, chemical and electrochemical stability, wide operating temperature range, non-volatility, nonflammability, environmental friendly, and cost effective. Electrolytes are classified into different types; aqueous (acidic, alkaline and neutral) electrolytes, organic/ionic-liquid electrolytes, solid-state/quasi-solid-state (solid polymer, gel polymer) electrolytes, which are commonly used in supercapacitors. Out of all these electrolytes, gel polymer electrolytes (GPEs) have drawn a lot of interest due to various advantages i.e. high ionic conductivity comparable to the liquid electrolyte, no leakage problem, no requirement of extra separator, good thermal and mechanical stabilities. Flexible nature of the GPEs makes it suitable for their use in flexible energy storage devices. GPEs comprises of aqueous or organic/ionic-liquid electrolytes that are entrapped in host polymer matrix. Commonly used host polymers for preparation of GPEs are; poly(ethylene oxide) (PEO), poly(methyl methacrylate) (PMMA), polyvinyl alcohol (PVA), poly(vinylidene fluoride-co-hexafluoropropylene) (PVdF-HFP), polyvinylpyrrolidone (PVP), polyacrylonitrile (PAN), etc. In the recent past, another innovative strategy has been adopted to improve the specific capacitance, and hence the specific energy of carbon supercapacitors, wherein a redoxactive species is directly added in to the liquid electrolytes or in GPEs. The redox reaction(s) involving fast charge-transfer in redox-additives at the electrode-electrolyte interfaces contribute to enhance the specific capacitance via additional pseudocapacitance and hence, energy density of the supercapacitors. Different redox-additives namely; lithium iodide (LiI), sodium iodide (NaI), potassium iodide (KI), rubidium iodide (RbI), Cesium iodide (CsI), hydroquinone (HQ), vanadium oxide sulphtae (VOSO4), p-phenylenediamine (PPD), methylene blue (MB), trimethyl-sulfoxonium iodide (TMSI), 1-butyl-1-methylpyrrolidinium bromide (BMPBr) and many more have been reported to add in electrolyte compositions to enhance the performance of supercapacitors. Redox-active electrolytes are further classified into four types; (i) aqueous redox-active

electrolytes, (ii) organic redox-active electrolytes, (iii) ionic-liquid redox-active electrolytes, and (iv) redox-active gel polymer electrolytes. viii The present thesis work focuses on the fabrication and characterization of carbon-based quasi-solid-state supercapacitors using activated carbon derived from waste-biomass pollen-cone with ionic-liquid based gel polymer electrolyte (ILGPE), and aqueous and non-aqueous ionic liquid based redox-active gel polymer electrolytes (R-GPEs). Performance of supercapacitors have been compared with the divices fabricated with neutral aqueous electrolyte (1M Na2SO4). The ILGPEs/R-GPEs and carbon-electrode materials have been characterized via different physical and electrochemical techniques. The electrode materials used in the fabrication of supercapacitors are activated carbons derived from waste-biomass pollen-cone activated by using two different activating agents ZnCl2 (ZAC) and KOH (KAC). Commercial activated carbon (CAC) has also been used as control electrode material. All the studies are chapter–wise summarized in the following sections. Brief introduction about the electrochemical energy storage devices, specially focused on supercapacitors, has been given in Chapter-1. The charge-storage mechanism of the different types of supercapacitors namely; electrical double layer capacitors (EDLCs), pseudo- or redox-capacitors and hybrid capacitors are also given. Details on the different type of electrode materials (carbon materials, metal oxides, conducting polymer etc.) and various electrolytes (aqueous, organic, ionic-liquid, quasi-solid-state) electrolytes for supercapacitor are also provided in this Chapter. The detailed description of preparation of porous activated carbons derived from wastebiomass pollen-cone (using two different activating agents, ZnCl2 and KOH) as a potential electrode material for supercapacitors and the preparation methods of various electrolytes namely; (PVdF-HFP/EMITFSI), non-aqueous redox-active gel polymer electrolytes PVdF-HFP/EMITFSI/KI and (PVdF-HFP/BMPTFSI/BMPBr, and aqueous redox-active gel polymer electrolyte (PVA/EMICl/TMSI) have been provided in Chapter-2. This is followed by the preparation of the electrodes and fabrication of the carbon supercapacitors/EDLCs. Various physical characterization techniques namely; X-Ray diffraction (XRD), Raman spectroscopy, Fourier transform infrared (FTIR) spectroscopy, field emission scanning electron microscopy (FESEM), tensile testing and thermal techniques vis. modulated differential scanning calorimetry (mDSC), thermogravimetric analysis (TGA) were used to study the properties of the activated ix carbon and gel polymer electrolytes. The electrochemical properties of the electrolyte materials and supercapacitor devices were characterized using different electrochemical techniques namely, electrochemical impedance spectroscopy (EIS), linear sweep voltammetry (LSV), cycling voltammetry (CV) and galvanostatic charge-discharge (GCD), as described in this chapter in detail. An optimization of activated carbons (ACs), derived from waste-biomass pollen-cone powder with different weight ratios of activating agents, has been performed by porosity analysis, as presented in Chapter-3. The AC-powders have been characterized via XRD, SEM, Raman and FTIR spectroscopy. The electrochemical performance of AC-electrodes have been tested by fabricating symmetric configuration of EDLCs with neutral aqueous electrolyte (1M Na2SO4) and quasi-solid-state ionic liquid incorporated gel polymer electrolyte (ILGPE). The free-standing film of ILGPE, comprising IL 1- ethyl-3-methyl imidazolium bis(trifluoromethyl sulfonyl)imide (EMITFSI), immobilized in a copolymer poly(vinylidine fluoride-co-hexafluoropropylene) (PVdFHFP), is found suitable as EDLC electrolyte due to its flexibility, high ionic conductivity and wide electrochemical stability window. Comparative performance of EDLCs, fabricated with AC-electrodes (activated using ZnCl2 and KOH) with aqueous liquid electrolyte and ILGPE, have been tested using CV, EIS, and GCD studies, presented in this

chapter. Performance of pollen-cone derived AC-electrodes has also been compared with commercial AC and un-activated pollen-cone carbon-electrodes. The effect of porous electrodes with both (aqueous and gel polymer) electrolytes on the performance of the EDLCs have been thoroughly discussed in this chapter. A non-aqueous, IL-based redox-active GPE has been prepared by immobilization of a combination of an IL 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide (EMITFSI) and a redox-additive potassium iodide (KI) in a host polymer PVdF-HFP as described in this chapter. Structural, thermal and electrochemical characterization of the GPE has been presented based on XRD, FTIR, TGA/DSC, ionic conductivity and electrochemical stability measurements. To assess the suitability of the redox-active GPE-film in supercapacitor applications, it has been employed as a quasi-solid flexible electrolyte in EDLCs, assembled with pollen cone-derived AC-electrodes. The effect of redox-additive KI on the supercapacitor's performance has been studied by comparative x EIS, CV, GCD tests. The GCD measurement have also been carried for large number of cycles followed by self-discharge tests on supercapacitor cells containing GPE films (with and without KI). The application of KI-incorporated redox-active non-aqueous GPE is found to substantially improve the overall performance of the supercapacitor, particularly, the specific capacitance (~250 F g -1) and energy (~35 Wh kg-1) with cycling performance up to 10,000 cycles. High energy density carbon supercapacitor of a wide potential window (~3.5 V) has been presented in Chapter-5, fabricated with symmetrical AC-electrodes and flexible GPE film composed of the ionic liquid (BMPTFSI) added with a redox-additive (BMPBr), immobilized in PVdF-HFP. The redox-additive BMPBr is also an ionic liquid, which has been added strategically in the IL-incorporated GPE to increase the interfacial redox-activities by introducing a redox-active species (Br-) in the electrolyte, maintaining high thermal and electrochemical stability of the supercapacitor. Suitability of GPE-film as the redox-active electrolyte for carbon supercapacitor is tested via mechanical, thermal and electrochemical measurements. The performance characteristics of the carbon supercapacitors with redox-active gel polymer electrolyte (R-GPE, containing redox-additive BMPBr) has been compared with GPE (without BMPBr) using various electrochemical measurements, viz., CV, EIS, and GCD measurements over prolonged cycles. The experimental results indicate an excellent impact of BMPBr-additive in the GPE composition on the characteristics of supercapacitor cells, such as specific capacitance (~250 F g -1), specific energy (~105 Wh kg-1) and their cyclic performance up to 10,000 cycles. Synthesis of an aqueous redox-active GPE (R-GPE) has been reported by adding a redox-active salt (trimethyl-sulfoxonium iodide, TMSI) in an ionic liquid (1-ethyl-3- methylimidazolium chloride, EMICl), and immobilized in a host polymer poly (vinyl alcohol) (PVA) as presented in Chapter-7. The free-standing film of R-GPE shows high flexibility and excellent electrochemical properties including high room temperature ionic conductivity (1.54×10-2 S cm-1) and wide electrochemical stability window (~2.9 V vs. Ag/Ag+), which makes the R-GPE film suitable for supercapacitor application. Two supercapacitors are fabricated using GPEs (without and with TMSI) and activated carbon electrodes, derived from a bio-waste pollen-cone. The performances of the xi supercapacitor cells were studied using different electrochemical characterization techniques like EIS, CV, and GCD tests. Presence of TMSI as redox-additive in R-GPE enhances the performance of the device in terms of specific capacitance (~613 F g-1) and specific energy (~69 Wh kg-1) as compared to the device with GPE (without TMSI). The supercapacitor cell with R-GPE demonstrates a moderate rate capability. The device offers good cyclic performance with high Coulombic efficiency up to 5,000 GCD cycles.

Contents

13. JAIN (Chakresh)
Development of silicon Sensors for Particle Detection in High Energy Physics Experiments.
Supervisor: Prof. Kirti Ranjan and Prof. Ashutosh Bhardwaj
Th 27174

Abstract

Silicon sensors in different configurations are widely used in various high Energy Physics experiments. Owing to several advantages offered in terms of the precision measurements of position energy and time response of traversing particles silicon sensors are presently employed in all four major experiments of the large hadron collider at CERN CMS ATLAS ALICE and LHC and are also proposed to be used in the future upgrades. High luminosity as well as in proposed lepton colliders. However the increased luminosity in these experiments for improved statistical precision results in a large multiplicity of charged and neutral hadrons viz pions protons neutrons etc. While the charged particles populate the radiation environment at the inner layers of the tracker neutrons being neutral long lived and having limited interactions constitute significant flux in the calorimeters and outer parts of the tracker. Due to such unprecedented harsh radiation environment radiation damage of silicon sensors in these experiments poses a major challenge for their reliable operations. The silicon sensor development campaigus are assisted by exploiting TCAD simulations for fabrication choice of polarity and design aspects. Efforts have been invested in studying the effects of radiation damage on these detectors caused due to both charged and neutral hadron irradiation. A radiation damage model for proton irradiation was developed earlier using TCAD tools, however a similar model for neutron irradiation was missing. The development of radiation damage models can also be used for design optimization of novel radiation hard silicon sensors. Furthermore, once the silion sensors are fabricated then stringent tolerances are imposed on their proper ties to maintain efficient physics performance. This requires these sensors to be extensively tested under temperature and humidity-controlled environment for their qualification.

Contents

14. Lamichhane (Shiva)
BFO/WO3 Bilayer Structure for Multifunctional Device Applications.
Supervisor: Prof. Arijit (Chowdhuri)
Th 26846

Abstract

Worldwide scientists are actively engaged in researching innovative materials exhibiting multiple functionalities in a single device structure. Researchers are involved in developing materials with enhanced functionality for futuristic multifunctional devices. Generally devices whose functional is related with their electrical magnetic and optical properties are termed as functional devices. Materials which exhibit two or more primary ferric properties simultaneously are termed as multiferroics. For the past few decades multiferroic materials have been explored for the fulfilment of criterion under multifunctional device applications. The primary ferroic properties of interest are ferroelectricity and ferromagnetism. Literature reports indicate that perovskites exhibit multiple properties of including piezoelectricity ferroelectricity ferromagnetism and are quite abundant innature besides being resistant to corrosion. Rhombohedrially distorted perovskite is noted to be one of the most investigated materials in the past many years owing to its exclusive room temperature multiferroic properties. It has been reported that BFO exhibits remarkable properties like high polarization and magnetization at room temperature. BFO belongs to R3s space group and has lattice constants . BFO in bulk form has been found to exhibit feeble multiferroic behaviour because of its discrete spiral spins sttructur and fluctuations in Fe valency values which further restrict its useful applications. It has ben established that a slight tailoring of its composition and defects drastically change the properties of perovskite materials therefore a careful tuning of stoichiometry is envisioned to result in imporved properties. In regards to this the recent research trend has focused from bulk to thin film for the accomplishment of better response in functional devices.

Contents

15. MAHBOOB ALI
Investigations on Electronic Structure and Charge Transport Mechanism in Size Controlled Lithium Iron Phosphate and its Solid Solutions for Lithium-Ion Batteries.
Supervisor: Prof. Sevi Murugavel
Th 26847

Abstract

Fossil fuels were the main sources of energy during the first three industrial revolutions, and as a result, massive greenhouse gases were emitted, resulting in problems such as global warming and ecological degradation. Since the Paris Agreement in 2015, countries

have progressively turned to developing clean, low-carbon, pollution free and renewable energy technologies as a key component of their energy development strategy to reduce greenhouse gas emissions and deaccelerate global warming. New energy storage technologies have the potential to change the driving force of socioeconomic development. Renewable energy storage technology has become essential to the modern revolution. Numerous energy storage technologies have been developed successfully in recent years to fulfil the current demand. Nevertheless, the raising concerns about climate change, electric vehicles (EVs) as well as hybrid electric vehicles (HEVs) are being developed at a fast pace, and are expected to replace the traditional vehicles powered by gasoline. To enable a smooth transition to EVs from combustion engine-based vehicles, lithium-ion batteries (LIBs) are the critical technology. Owing to the high working voltage of LIBs, it possesses a low memory effect and high energy density compared to traditional batteries. LIBs are the dominant power source for a variety of portable electronic devices and are booming all over the world. However, the demand for higher energy and power capabilities with costeffective, sustainable and environmentally friendly materials, is rising for the same applications. The key components of LIB are the electrode material and electrolyte, which decides the overall electrochemical performances. Ever since the proposal of the olivine structure LiMPO4 (M = Fe, Mn and Ni) as a cathode material for lithium-ion batteries, LiFePO4 (LFP) has become one of the promising cathode materials in the field of battery research. In recent years, the considerable demands for high performance and safety along with climate concerns, the large-scale energy storage system in electric vehicles (EVs) and plug-in hybrid vehicles (HEVs) have inspired numerous research studies to optimize the LFP cathode material. The LFP possesses many interesting properties including high-open circuit potential (3.5 V), high theoretical capacity and cycling rates, low-cost, and non-toxicity. Despite having many fascinating electrochemical properties, the main drawback of LFP lies with its low gravimetric density and poor electrical conductivity (both electronic and ionic) which limits the lithium intercalation/deintercalation rates, and hence the practical specific capacity. In the last two decades, various strategies have been proposed for the synthesis of LFP with enhanced electrochemical performance characteristics such as high capacity and good cycling stability. Extensive research is being conducted on LFP for lithium-ion batteries to meet the demand of commercial applications. Different techniques have been used to improve the overall electrochemical performance, which includes carbon coating, reduction in the particle/crystallite size, solid solution and doping. Thus, we mainly focused on the study of electronic structure and charge transport in different LFP crystallite sizes, lithium content and Mn doping, which has a significant impact on enhancing its electrochemical properties. To investigate both electronic structure and charge transport different experimental techniques have been used. The most recent study on pristine LFP reveals that the polaron transport is strongly determined by its concentration, hopping length and activation energy. Therefore, it becomes crucial to understand the electronic structure of the LFP system since these physical parameters determine the polaron transport. Additionally, it becomes necessary to gain a fundamental understanding of the electronic structure of the LFP system by using an alternative experimental approach. The main objective of the present doctoral thesis is to study the electronic structure and charge transport mechanism of size-controlled LFP and its solid solutions. The different nanosized LFP samples have been prepared by a modified single step solid-state route. Similarly, we have prepared solid solution Li1-xFePO4 ($0 \leq x \leq 0.20$) samples by a twostep method in which synthesis of stochiometric LFP samples (by solid state route) followed by chemical de-lithiation by reacting it with an appropriate amount of potassium persulphate (K2S2O8)

in deionized water. Further, we have synthesized Mn doped LiFe1-xMnxPO4 with ($0.05 \leq x \leq 0.20$) solid solution samples with nanometer crystallite size (~ 45 nm). The various analytical techniques have been used to understand the structural and charge transport phenomena. Among these spectroscopic techniques, XAS recognized to be valuable tool for the analysis of the electronic structure of LFP and other related cathode materials. This technique provides chemical and elemental sensitivity due to its involvement of valence and core electrons, revealing strong electron correlation in the transition-metal (TM) 3d electron and hybridization characteristics between oxygen and TM valence state. More specifically, Fe L2,3 –edge (2p1/2,3/2 → 3d) XAS in soft X-ray region is very sensitive to probe the density of unoccupied states in the Fe 3d level. The sensitivity provided by the XAS technique leads to gaining information on complete electronic structure that is relevant to cathode material performance including valence, spin states and local structural effect on the crystal field. Further, the electrical conduction mechanism of different crystallite sized LFP specimens has been studied using ac impedance spectroscopy over a wide range of temperatures. The electrical conduction phenomena have been explained within the framework of the Mott model for Polaronic conduction. These studies bring out new information which would help in designing cathode materials with improved electrochemical performance characteristics in next generation LIBs. In the first section, we address the synthesis and characterization of size dependent LFP samples using the modified solid-state route method. We made an attempt to investigate the electronic and local atomic structure including site symmetry of Fe in olivine structured LFP with different crystallite sizes (CSs) and its effect on the electronic conductivity. The lattice parameters are found to contract with a decrease in CS, monotonically, whereas the electronic structure parameters exhibit two different regions with a threshold anomaly around 31 nm. More specifically, we present the results of a combined Mössbauer and X-ray absorption spectroscopy (XAS) to understand the electronic structure and local site symmetry of Fe in olivine structured LFP with different CS. The X-ray absorption spectra followed by charge transfer multiplet calculations revealed that the D4h point group accurately describes the symmetry of Fe ions. We have found that the local symmetry of Fe ions is well described by the D4h point group with intermixing between eg and t2g orbitals. Additionally, the evolution of Fe-3d and O-2p hybridization was monitored through the O K-edge XAS. These results revealed the change in bonding character between the Fe-3d and O-2p states with decreasing CS. Further, the temperature dependent dc conductivity has been investigated and analyzed by Mott's model of polaronic conduction, which exhibits non-Arrhenius behavior. At high temperatures, the scaling of the ac conductivity spectra with Summerfield scaling law was found to exhibit pronounced deviations. The scaling of the ac conductivity spectra at high temperatures has improved significantly by using the random barrier model predictions. We suggest that at high temperatures the number density of polarons increases with the temperatures. Additionally, we have prepared solid solution of Li1-xFePO4 ($0 \leq x \leq 0.2$) by a two-step method in which synthesis of stochiometric LFP samples (by solid state route) followed by chemical de-lithiation by reacting it with an appropriate amount of potassium persulphate (K2S2O8) in a deionized water. The presence of single-phase in Li1-xFePO4 solid solution has been demonstrated from the high-resolution x-ray diffraction method. Various analytical techniques have been used to understand the structural and charge transport phenomena in different solid solution Li1-xFePO4 compositions. The nanosized Li1-0.20FePO4 solid-solution was found to exhibit the highest polaronic conductivity with 7.71x10-8 S/cm, which is two orders higher than the bulk stoichiometric LFP. We made an attempt to understand the enhanced polaronic conductivity with the aid of unique

electronic properties, which have been explored by the combined use of Mossbauer and X-ray absorption spectroscopy techniques. Finally, we demonstrate the characteristic nature of solid-solution formation is closely linked with the host material crystallite size, defect concentration and morphology. Further, olivine structured LiFe1-xMnxPO4 with ($0.05 \leq x \leq 0.20$) were synthesized by the solid-state reaction. We have carried out detailed structural and charge transport investigations to examine the effect of Mn2+ substitution in LFP. The substitution of Mn2+ into olivine LFP leads to the formation of solid-solution and it exhibits monotonic expansion of unit cell volume due to its larger ionic radius. The increased unit cell parameters with Mn2+ addition is substantiated by the observed red-shift in the unique vibrational mode of Fe2+/Mn2+ -O revealed by Raman spectroscopy. In parallel, we used X-ray absorption spectroscopy (XAS) to unravel the electronic structure of LiFe1- xMnxPO4 solid-solution, where the substitution of Mn2+ has a significant contribution towards the lattice structure modifications and it acts as a stabilizer in the threedimensional framework structure. The simulated Fe and Mn L-edge XAS by using the ligand field multiplet theory suggest that symmetry reduction (Oh → D4h) takes place upon Mn2+ incorporation. In comparison with pure LFP, the impact of Mn2+ substitution on LFP structure results in a two-order enhancement in the polaronic conductivity. Additionally, the temperature dependent dc conductivity has been investigated and analyzed by using Mott's model of polaronic conduction. We correlate the enhanced polaronic conductivity in the LiFe1-xMnxPO4 solid-solution phase with the combined effect of increased polaron concentration, reduced activation energy and hopping length. The obtained favorable structural and charge transport properties underscore the superior performance of LiFe1-xMnxPO4 as cathode material in newer generations of rechargeable batteries.

Contents

16. Moditma

Facile Synthesis of Fe-Co Alloy Nanoparticles as potential Antibacterial Agents and Magnetic Fillers for Enhanced.

Supervisor: Prof. S. Annapoorni

Th 26848

Abstract

The present thesis work focuses on the synthesis and applications of FeCo nanoparticles. With the high saturation magnetization and permeability values, This alloy of metallic iron and cobalt has gained considerable interest in the recent past in various fields of biomedicine data storage for microwave absorption technologies in power generation sector and for nano composite exchange spring magnets. Here first an attempt is made to synthesize highly magnetic uniform nanoparticles of FeCo and understand the evolution of fundamental properties across different alloy compositions. The equiatomic alloy composition is then chosen to investigate their usability in two sectors. Namely as potential antibacterial agents and secondly as magnetic fillers to enhance electromagnetic absorption in the microwave frequency range. The various attempts to synthesize

FeCo nanoparticles with the desired structural and magnetic properties in the equiatomic composition range have been presented in two reducing agents namely sodium borohydride and ethylene glycol have been used for this purpose. The following could be concluded for the material properties obtained using the different approaches.

Contents

17. PANDEY (Anand)
Search for Exotic Nuclear Shapes at High Spins in Neutron Deficient Xe a nd I Nuclei with Mass A< 120.
Supervisor: Prof. S.K. Chamoli
Th 26850

Abstract

The present thesis investigates the nuclear shapes at high spins in neutron deficient nuclei, specifically 118Xe, 117I, and 115I isotopes having mass A < 120. The experimental study involves γ-ray spectroscopy and lifetime measurements to study the structural features in the nuclei. In mass A ∼ 120 region, the proton, and neutron Fermi surfaces lie near the low-K and high-K orbitals of the h11/2 sub-shell, respectively, which lead to different shape driving properties in these nuclei. The experiment was done with the 15-UD pelletron accelerator facility available at the Inter-University Accelerator Centre (IUAC), Delhi. The high spin states in the nuclei of interest were populated with 93Nb(28Si, xpynγ) reaction at 115 MeV beam energy. The de-exciting γ-rays were detected using the Indian National Gamma Array (INGA), consisting of clover detectors. The spectroscopic study of 118Xe nucleus resulted in several new γ-transitions, confirmation of negative parity of an octupole correlated band with polarisation asymmetry measurement, more precise data on the B(E1) values for the octupole correlated γ-ray transitions, etc. The lifetimes of three excited states of the yrast band in 118Xe were measured using the Doppler shift attenuation method. Comparison of experimental B(E2) and Qt values with theoretical model-dependent calculations suggested a significant decrease in the deformation in the yrast configuration after the first band crossing. A dip in the Qt values at a rotational frequency of 0.39 MeV was attributed to two-neutron alignment and loss of collectivity. Overall, the experimental results were consistent with theoretical predictions. In the case of 117I, the DSAM technique was used for the first time to measure the lifetime of excited states in the negative parity band. The extracted B(E2) and Qt values show a decreasing trend with increasing spin, indicating a loss of collectivity. The results of the theoretical TPSM calculations tend to support this observation too. The observed loss of collectivity with the increasing spin in the present experiment thus confirms the loss of collectivity suggested as, one of the main reasons for the observed band termination beyond Iπ = 43/2− $\hbar$ spin state in this negative parity yrast band in 117I. In the present thesis work, 115I nucleus was

studied with DSAM lifetime measurements for the first time. In the measurements, the mean lifetime of six high spin states has been obtained. The extracted Qt values, when plotted as a function of spin values, show a decreasing trend with xxii Abstract increasing spin, suggesting a loss of collectivity. The experimental results show loss of collectivity at high spins after the bandcrossing rather gradually. The results of the TPSM calculations are perfectly in agreement with the experimental findings. However, in contrast to the abrupt loss of collectivity observed in 117I, the collectivity in 115I gradually decreases as the spins increase at high spin values. The experimental observation in the present work are perfectly in line with the suggestions made in earlier spectroscopy works for explaining the band termination behaviour.

Contents

18. PARVEEN KUMAR
Metal Oxides Based Hydroelectric Cells as Green Energy Source.
Supervisor: Dr. Vivek Kumar Verma
Th 26851

Abstract

Most of the time, problems with environmental pollution are amplified by energy production. Hence, there has been a search to develop novel green energy source and technology alternatives. Notwithstanding their inherent environmental contamination issues, coal and crude oil are currently the most widely used energy sources. Because it is so pervasive, severe environmental pollution is negatively harming people's health. To safeguard the environment, it has become vital to create and implement new energy alternatives. Because of the world's diminishing crude oil reserves, using electric vehicles (EV) in place of gasoline-powered vehicles is currently seen as a potential future for mass transportation. Unfortunately, the use of lithium-ion batteries and other components in EV technology will result in significant amounts of hazardous chemical and electronic waste. As a result, the introduction of such innovative technical solutions for the public transit system will result in yet another tragic circumstance. Thus, it is now more important than ever to develop innovative environmentally friendly green energy alternatives. In this regard, the groundbreaking Hydroelectric Cell is a promising green energy device with many benefits for humanity. A device that can produce electricity using only a few droplets of water at ambient temperature without the use of any external power or chemicals. The Hydroelectric Cell (HEC) is a device that can produce about a quarter ampere current at less than 1 V. These cells can be combined to produce enough power to run LED lights and electric fans. Although, the development of HEC is in its early stage. There are several challenges to use this device at commercial level. Overall, it seems promising invention for green energy production. The objective of this thesis work is to investigate hydroelectric cell with efficient electrical power generation. Using this innovative gadget known as a hydroelectric cell, energy can be produced with no emissions of carbon dioxide. The present work includes hydroelectric cells made of different metal oxides offer a unique, inexpensive, and environmentally benign source of

green energy with practically no ongoing costs. Without the release of any toxic emissions, eco-friendly electricity has been produced from metal oxides using just microscopic amounts of water. Also, in xi this thesis, the focus is on the production of large and sustainable amount of green electrical power. The studies presented involve a wide variety of characterization techniques such as structural, morphological, spectroscopic, along with hydroelectric properties. Chapter 1 includes the ideas connected to the hydroelectric cell, metal oxide/ferrite, and their general and fundamentals. It has been discussed how different kinds of materials interact with water molecules. The types of metal oxides and ferrites have been briefly reviewed. In this chapter, the significance of green energy is also discussed. Motivation for this study and a brief work plan for the thesis have been given in this chapter. Thorough literature review of the hydroelectric cell has been composed in chapter 1. Chapter 2 outlines various experimental methods that have been employed to synthesis and analyze the prepared samples, along with the pertinent theoretical underpinnings. Porous materials have been attracted to researchers because of their unique characteristics. Mesoporous materials play a significant role among them. These materials can be employed for a variety of purposes, including heterogeneous catalysis, gas storage, gas separation, heavy metal ion adsorption, optoelectronics, sensing, drug delivery, magnetism, and energy applications, thanks to their resilient nature, tunable porosity, and surface activity. First, several processes that are typically utilized to synthesize materials such as hydrothermal, solid state, co-precipitation, micro-emulsion, sol-gel, etc. are briefly addressed. Characterization methods used to examine prepared samples, such as powder X-ray diffraction, SEM, FT-IR, BET, dielectric/impedance analyzer, XPS etc., are presented in depth. Chapter 3 deals with the synthesis of pure and K doped $MgFe_2O_4$ based hydroelectric cells with mesoporous structure and good chemical stability by solid-state sintering method. Using this innovative gadget known as a hydroelectric cell, energy can be produced with no emissions of carbon dioxide. The structural and phase analysis of prepared samples were investigated using Rietveld analysis of powder X-Ray data. Surface morphology of all samples were examined by using FESEM. By measuring the dielectric and dc conductivity of all the samples in both dry and wet states, it was xii possible to further explore the dissociation of water molecules and the conduction of dissociated ions. The hydroelectric cell based on $Mg_{0.9}K_{0.1}Fe_2O_4$ showed the highest output power. Offload current and open circuit voltage have been recorded for prepared cells of $Mg_{1-y}K_yFe_2O_4$ ($0 \leq y \leq 0.3$) samples, with spray of few milliliters of water on these cells. Open circuit voltage for all the samples was found in the range 944 - 965 mV while the maximum offload current was found in the range of 13.9 – 34.8 mA. Furthermore, offload current was investigated for 2 hours after spray of water and it was found that value of current decreases with time. It was observed that offload current of pure $MgFe_2O_4$ sample improved from 13 mA to 34 mA for $Mg_{0.9}K_{0.1}Fe_2O_4$ sample. Further doping of K in $MgFe_2O_4$, offload current decreases to the value of 25.4 mA and 18.4 mA for $Mg_{0.8}K_{0.2}Fe_2O_4$ and $Mg_{0.7}K_{0.3}Fe_2O_4$ samples respectively. Chapter 4 presents the synthesis of porous SnO_2 samples for hydropower cells in order to achieve good quality material for hydroelectric properties by solid state sintering method. The X-ray diffraction pattern utilising Rietveld analysis supported the phase formation and structural analysis of the sample. Field emission scanning electron microscopy was used to analyse the sample's surface morphology. Using image j software, the average grain size of the porous material was shown to be 65 nm. The Barrett-Joyner-Halenda method was used to evaluate the SnO_2 nanoparticles' pore size distribution and specific surface area of

prepared samples. To investigate the hydroelectric properties, a circular pellet with a diameter of 2 inches (PK1) and a square pellet with a side of 2 cm (PK2) were fabricated. The peak current and voltage values for the square pellet (PK2) were 12.5 mA and 0.972 V, respectively, while the peak current and voltage values for the circular pellet (PK1) were 72.1 mA and practically constant voltage of 0.981 V. Utilizing sample dielectric and DC conductivity behaviour, the dissociation of water and conduction phenomenon have been verified. When water is sprayed on SnO2 disc, some amount of water adsorbed by chemisorption. The edges of grains work as activated sites of the surface which help in dissociation of water molecule and form hydroxyl groups. These hydroxyl groups get attached with metal cations. At the second stage, after chemisorbed layer, subsequent water molecules interact physically on the first formed hydroxyl layer. To xiii investigate the power production properties of SnO2 cell, we have taken the observations of voltage and current for the samples PK1 and PK2 for 1 hour after spray the deionized water on samples. Measurements were repeated in same sample as well in different sets of samples to observe the consistency/reproducibility of results. SnO2 based Hydroelectric cell delivers maximum power ~71.8 mW in 19.63 cm 2 area of SnO2 cell (PK1) with peak short circuit current 72.1 mA, approximately 4 times higher than reported 17 mA current in ferrite-based HEC. Production of voltage and current in HEC is mainly depending on the dissociation of water on the surface of the metal oxide and movement of dissociated ions in the material. Chemi-dissociation process predominantly depends on the electronegativity of the metal cations, defect sites and porosity in the microstructure. The movement of dissociated ions in material depends on internal resistance, grain boundary nature, water molecule dissociation capability and porosity of the medium. Chapter 5 comprises a simple, cost-effective, and two-stage solid-state sintering approach to prepare lithium-doped SnO2 hydroelectric cells with high efficiency and sustainability in comparison to pure SnO2 hydroelectric cells. The X-ray diffraction technique and field emission scanning electron microscopy were used to analyze the morphological behaviour and structural makeup of the synthesized samples. According to SEM pictures, all samples show porosity with the average grain size falling between 45 and 55 nm. Using the Barrett-Joyner-Halenda approach, pore volume, pore size distribution, and adsorption-desorption isothermal curves were studied. Dielectric and dc conductivity tests of samples in both dry and hydrated conditions have proven that the dissociation of water molecules into H3O + and OHions and subsequent ionic diffusion of these dissociated ions for the electrical power production inside the material. To study the hydroelectric capabilities, 2 inch-diameter round pellets of pure and Li-doped SnO2 samples were created. It was discovered that the 15 mol% Li doped SnO2 sample had a nearly constant current of 70 mA and a voltage of 0.98 volts for a significant amount of time. Thus, because of their high surface-to-volume ratios, excellent charge transport capabilities, and advantageous physiochemical properties, these nanostructured materials can serve as effective and attractive options for green energy production devices. Maximum current obtained in pristine and Li doped SnO2 sample is almost same but that xiv current is more sustainable in Li doped SnO2 samples for almost 2 hrs. Sustainable and enhanced response of current in doped samples can be primarily attributed to the alkaline Li+ bonding interface to build a sturdy adhesion to H2O molecules and porosity which can efficiently induce more dissociation of water molecules. It is observed that the current generated in 15 mol% Li doped SnO2 HEC reduced to 11 mA from 71 mA in 2 hrs. Decrease in current may be attributed to concentration loss and oxidation of zinc electrode. Chapter 6 describes the solid-state

approach which was used to create alkali (Na, K) doped tin oxide nano porous structured hydroelectric cells. To establish the phase formation of the samples, X-ray diffraction and Fourier transform infrared spectroscopy analyses have been carried out. Using field emission scanning electron microscopy, the surface morphology of each sample was examined. With the use of the Barrett-Joyner-Halenda procedure, the samples' mesoporosity was verified. A maximum output power of 61.5 mW was discovered to be provided by 5 Mol% K doped SnO2 HEC after hydroelectric properties of round pellets with a diameter of two inches were investigated. Compared to pure SnO2 HEC, the observed electricity generation in doped SnO2 samples is more consistant. By measuring the dielectric and dc conductivity of all the samples in both the dry and wet states, it was possible to further explore the dissociation of water molecules and the ionic conduction of dissociated ions. Alkali element doped tin oxide nano porous structured hydropower cells can be used as an unconventional source of energy, according to results that have been observed. It can be analyzed that maximum current obtained in pure and alkali (Na, K) SnO2 sample is almost same but that current is more sustainable in alkali (Na, K) SnO2 samples for almost 2 hrs. Maximum output power of 61.5 mW was delivered by 5 Mol% K doped SnO2 HEC. The sustainability in the current of doped samples can be primarily attributed to the alkaline bonding interface to build a sturdy adhesion to H2O molecules and porosity which can efficiently induce more dissociation of water molecules. Decrease in current with time may be attributed to oxidation of zinc electrode and concentration loss. Chapter 7 deals with the synthesis of WO3 loaded SnO2 nanocomposite hydroelectric cells by using solid state technique. Powder X-ray diffraction, a scanning electron xv microscope, and Fourier Transform Infrared spectra were used to examine the structural, morphological, and hydroelectric properties of the nanocomposites. Using the Barrett-Joyner-Halenda approach, adsorption-desorption isothermal curves, pore size distribution, and pore volume were examined. By measuring the dielectric and dc conductivity of all the samples in both dry and wet states, it was possible to analyze the ionic diffusion of the dissociated H3O + and OHions. The monoclinic WO3 phase and tetragonal SnO2 phase of the biphasic composite are validated by the powder Xray diffraction pattern. Utilizing an X-ray photoelectron spectrum, surface chemical analysis and oxygen defect investigation were explored. SEM micrographs showed the homogeneous grain distribution and well-crystalline shape. To examine the hydroelectric capabilities, circular cells of WO3 loaded SnO2 nanocomposite samples with a 2-inch diameter have been used. The highest short circuit current, open-circuit voltage, and off-load output power of the manufactured HEC of 19.63 cm2 area of 10 Wt% WO3 loaded SnO2 nanocomposite are 655 mA, 0.959 V, and 628 mW, respectively. The WO3 - SnO2 nanocomposite-based hydroelectric cell has a significant output power and has emerged as a workable green energy source. It was observed that maximum current value is obtained in 10 Wt % WO3 loaded SnO2 nanocomposite sample is 655 mA which is the highest value as reported in literature so far. This enhanced response of current in WO3 loaded SnO2 nanocomposite samples in compared to pure sample can be primarily attributed to increase in water dissociation capability due to more oxygen vacancies generated in the sample. Also, tungsten oxide dehydrate is examined to have low activation energies for bulk and very high proton conductivity in temperature range 273-423 K. Groutthus phenomenon contributes to proton diffusion in this compound due to the existence of layered water in the crystal structure of tungsten oxide dehydrate. As a result of this generation of large amount of current takes place in WO3 loaded SnO2 nanocomposite samples as compared to pure SnO2 sample. The decrease in the value of

current with the passage of time may be attributed as oxidation of zinc electrode and concentration loss. It is very challenging to modify these problems for the preparation of more efficient HECs. xvi Chapter 8 provides a summary of the findings reported in chapter 3 to chapter 7 and comparison with available literature on Metal oxide based hydroelectric cell. This chapter also include the future scope of research and challenges. The study of hydroelectric properties has been accomplished in order to achieve efficient metal oxides with variation in variation parameters such as: • Selection of various metal oxides to explore suitable for adsorption and dissociation of water molecules in view of hydroelectric application. • Doping of different monovalent ions in the metal oxides to create suitable microstructure, which is helpful to enhance hydroelectric power generation. • By tuning the porosity in metal oxides dissociation process as well as conduction of dissociated ions have been modified significantly. • Nanocomposite materials also explored for better hydroelectric properties.

Contents

19. SAINI (Lalit Kumar)
Interactions of Dark Matter with Color Multiplets.
Supervisor: Prof. Sukanta Dutta and Prof. V. Ravindran
Th 27175

Abstract

Nature has been very kind to us as the various phenomena happening around us can be explained by simple science rules. High energy physics experimentalists have been rigorously working to get more and more data on the small scale physics. Over the time this data has strengthened our belief in the standard model of particle physics. The discovery potential of the experiments have increased in the past few years and with these advancements various discrepancies have been observed such as the neutrino mass low energy anomalies missing matter content dark energy. A number of beyond the SM scenarios have been proposed to explain these experimental discrepancies. These models predict interesting new physics effects which by far have not been observed thereby limiting the parameter space of these models. It can be argued that the new physics is either very weakly interacting or it is present at a very high energy scale. One of the biggest unexplained discrepancy is the missing mass problem observed at galactic to cosmological scales. Over the decades this problem which is designated as dark matter has shown up in rotation velocity curves of galaxy gravitational lensing power spectrum of cosmic microwave background big bang nucleosynthesis structure formation and recently in bullet clusters but still there is no established model to explain this. The most straightforward explanation for these observations suggests that this DM exists as a fundamental or composite particle from some BSM physics. Futher observations suggests that this particle is neutral under electromagnetic as well as color charges stable and non-relativistic.

Contents

1. Motivation and introduction 2. Dark matter interactions induced by scalar and pseudo-scalar portal. 3. Model independent dark matter interactions with top/bottom. 4. Dark matter searches at LHC using effective field theories. 5. Summary and conclusion.

20. SETHY (Pradyumna Kumar)
Phenomenological Studies on High Energy Physics.
Supervisors: Prof. S. Somorendro Singh
Th 26852

Abstract

The creation of magnetic field in relativistic heavy ion collision and its influence on the dynamics of charged particles quarks is inevitable. Magnetic field causes non trivial effects on the collective excitation of the thermal system. The dynamics of electrically charged particles in the strong magnetic field would be effectively on dimensional because they tend to move along the magnetic field. Dimensional reduction from 3 spatial to 1 spatial direction. Thus the rotational invariance of the space of the system is broken since the particles tend to get aligned along the direction of magnetic field. Adhering to the concepts of quantum mechanics and cooper theorem in solid state physcis in such situation of dimensional reduction in spatial dimension a weak interaction of particles load to pair formation. Quarks and antiquarks pair more effectively in strong magnetic field. The dilepton production rate is calculated by considering the MEQM. Quasi particle model and modified effective quark mass is suitably used to accommodate the impact of intense magnetic field on the exotic state of matter. A modest enhancement in the dileption yield is observed by incorporating the non zero value of quark mass dependent on non zero chemical potential and magnetic field. This enhancement in the yield has been prominent at low and intermediate energy which is consistent with the recent work by Tuchin. We used a suitably modified magnetized effective quark mass to calculate the dilepton yield. Our model results are in good quantitative agreement with the recently reported results. The study focussed on the dilepton yield for variable magnetic field ranging from and also for zero and non zero chemical potentials. The dilepton yield is found to be increasing with the increase in magnetic field and also with the increase in chemical potential. The main results of our work essentially emphasizes on the dependence of dilepton yield from magnetized quark gluon plasma on the magnetic field and the chemical potential. Theses results may be useful to discover the properties of QGP in the heavy ion collision experiments.

Contents

1. Introduction. 2. Phenomenological models and quasi particle model. 3. Dilepton production from OGP with dynamical quark mass in heavy ion collision. 4. Photon production rate from OGP with dynamical quark mass in heavy- ion collision. 5. Dileption production from OGP in the background magnetic field in heavy-ion collision. Summary.

21. SINGH (Manvinder Pal)
Dark Matter Scenarios in Extended Scalar Sector.
Supervisors: Prof. Sukanta Dutta and Prof. Mamta
Th 26853

Abstract

In this thesis, we have attempted to address the nature and detection of viable DM candidates in the lipophilic two higgs doublet model extended by a singlet scalar and in gauged model scalar extension. We briefly discuss the SM and its unresolved issues in chapter first chapter. Next we briefly introduce dark matter and discuss its current detection techniques. The second chapter is based on the article where we study the modified contribution to the coherent elastic neutrino nucleon scattering cross section resulting from the inclusion of an extra SM singlet complex scalar field. We invoke additional gauged symmetry, which facilitates the introduction of the new neutral gauge boson Z. The coupling of Z with leptons in the model facilitates the scattering of neutrinos with the nucleus via Z-Z and Z-Y mixing induced by the charged lepton loops. To investigate the significance of new physics effects in the models we look for a variation in the CEvNS crossection compared to the SM one corresponding to the parameter region allowed by experiments such as borexino texono CHSRM and COHERENT. We find that the model with symmetry enhances the cross-section appreciably in comparison to those models with and symmetries. We further investigate the neutrino floor sensitivity for upcoming XENONnT and super CDMS direct detection experiments.

Contents

22. SUMIT KUMAR
Electromagnetic Shielding Studies of Magnetic Nano-Ferrites Based Composite Materials.
Supervisor: Dr. Vivek Kumar Verma
Th 26854

Abstract

Summarizes the results obtained in the present investigations on electromagnetic Shielding studies of magnetic nano ferrites based composite materials and future course of work on present investigations. The electromagnetic shielding studies have been accomplished in order to achieve efficient shielding materials with variation in various parameters such as in the present thesis an effort has been made to understand the effect of magnetic materials including soft and hard ferrites as various fillers for shielding materials and role of their magnetization and thinkness on the microwave shielding materials based on magnetic nanoparticles based composites with various host matrices such as polyaniline grapheme oxide multiwaalled carbon nanotubes and two dimensional titanium carbide have been done. The present work includes synthesis of magnetic fillers and their dispersion in mixed conducting polymer nanocomposites. A series of multi component composites have also been done. The present work includes synthesis of magnetic fillers and their dispersion in mixed conducting polymer nanocomposites. A series of multi component composites have also been synthesized which comprise to two different properties in the fillers and their effect on the shielding properties have been studies. Also in this thesis the focus is on absorption based electromagnetic radiation shield materials. The studies presented involve a wide variety of characterization techniques such as structural morphological spectroscopic thermal along with shielding effectiveness.

Contents

1. Introduction. 2. Method of synthesis and characterization techniques. 3. Electromagnetic shielding response of spinel ferrites AFe2O4 (A=Ni, Co and Zn) embedded into polyaniline matrix. 4. Modified magnetic properties of Zn doped nicket ferrites and shielding response of their composites with PANI. 5. Highly efficient shielding composites comprised of Co1-xZnxFe2O4 and PANI and their deposition over fabrics to control EM interference. 6. EM radiation pollution control by hybrid composites consist of ferrite nanoparticles and carbon-based derivatives. 7. Introduction fo 2D MXene material with ferrite nanoparticles and multiwalled carbon nanotubes resulting highty effective shielding materials. 8. Conclusions. Publications.

23. VANDANA
Realization of Multicomponent Materials and Flexible Devices for Energy Applications.
Supervisor: Prof. *Brajesh Chandra Choudhary*
TH 27179

Abstract

Growth of modern civilization and rapid industrialization has led to indiscriminate use of fossil fuels. With the increasing population energy requirements are also increasing to fulfill the growing demands resulting in energy crisis. Large scale use of vehicles and unthoughtful and wasteful use of energy resources in the present and past has exhausted most of the non renewable resources. This has resulted in various energy problems like depletion of fossil fuel supply and oil resources. One of the possible solutions towards this serious problem is the energy harvesting where waste energy is utilized in useful work so that the dependence on traditional energy sources could be reduced to some extent. Harvesting energy from the renewable sources such as solar wind hydrothermal geothermal mechanical thermal and electromagnetic energies ona large scale can fulfill the energy requirements of mankind to some extent in terms of powering essential electronic appliances. Amongst all the available energy harvesting technologies harvesting solar thermal and mechanical energies has gained a lot of interest because of easy availability in environment. Hence the present thesis work focuses on the energy harvesting using thermal solar and mechanical source of energy. In order to meet all these requirements a multifunctional material is required to be identified which could be utilized as an efficient energy harvester having the capability of harnessing solar thermal and mechanical energies. These multifunctional materials must possess good ferroelectic pyroelectric and piezoelectric properties. Among all the multifunctional lead zirconium titanate and lanthanum doped lead zirconium titanate films are the best candidates because of their remarkable values of pyroelectric coefficient piezoelectric coefficient and remnant polarization for development of efficient thermal mechanical and solar energy harvesters. Moreover such devices can also be transformed into flexible devices making them more useful and advantageous in day to day life.

Contents

1. Introduction, literature survey and outline of thesis work. 2. Growth and characterization techniques. 3. Structural and electrical characterization of pure and doped lead zirconium titanate (PZT) thick films. 4. Pyrroelectric properties of pure and doped lead zirconium titanate (PZT) thick films for thermal energy

harvesting applications. 5. Fabrication and characterization of ferroelectric photovoltaic device based on pure and doped PZT thick films. 6. Thermal and mechanical energy harvesting using pure and doped PZT based flexible devices. 7. Conclusions and scope of future work.

24. VIKAR AHMAD
X-ray Based Investigation of Vacancy Transfer in Low Energy Heavy-Ion, Heavy-Atom Collisions: MO Picture.
Supervisors: Prof. Punita Verma and Prof. Samit Kumar Mandal
TH 26838

Abstract

Super heavy atomic systems with united atomic numbers far beyond existing matter have attracted many researchers years ago. Beyond the normal Dirac equation for a point charge cannot be solved. For the innermost electron levels even dive into the negative continuum due to tremendous relativistic effects. These superheavy systems can be approached in relatively slow heavy ion heavy atom collisions which are slow compared to the orbital velocity of the innermost electrons of concern. In such collisions the collision partners transiently form a quasi molecule or an united atom with atomic number as a sum of the atomic numbers of the collision partners being the atomic numbers of projectile and target respectively. The energy levels of the inner shells in such quasi molecules can be probed by creating vacancies through ion impact there and observing their decay by X-ray emission in the separated partners or in the quasi molecule itself simple perturbation treatment is insufficient to explain the vacancy creation as well as ionisation processes in these quasi molecules and are explored under the molecular orbital picture. According to MO picture the collisons with being the projectile velocity and orbital electron velocity of the asymmetry parameter lie in quasi adiabatic regime. When the projectile velocity is slow as compared to the orbital velocity of the target electrons the larget inner shell electrons continuously adjust themselves to the perturbation brought in by the slow moving ions which lead to the formation of quasi molecules transiently during the collsion.

Contents

25. VINEETA
Synthesis and Optical Spectroscopic Characterization of Two Dimensional MoSe2 and MoS2..
Supervisor: Prof. Shyama Rath
Th 26855

Abstract

Atomically thin two-dimensional TMDs represent an emerging class of materials with distinctive electronic and optical properties in the mono and few layers limit along with structural stability extraordinary physical and chemical properties. The aim of this work is to study and analyse the optical and thermal properties of two dimensional layered atomically thin molybdenum dieseline and molybdenum disulphide and are indirect band gap semiconductors with bulk bandgap values of respectively which change to a direct bandgap in their monolayer limit. The work of this thesis is broadly divided into two parts (1) understanding and

formulating the underlying growth mechanism of mono and few layers thick Nano sheets of MoSe2 and MoS2 via physica and chemical synthesis routes respectively secondly studying their layer dependent optical and thermal properties by optical spectroscopic techniqes namely UV-vis Raman and photoluminescence spectroscopy.

Contents

1. Introduction. 2. Experimental techniques. 3. Raman spectroscopic investigations of the selenization of MoO in the chemical vapour deposition process to form two-dimensional MoSe2. 4. Raman spectroscopic study of the layer-dependent davydov splitting and thermal conductivity of chemically vapour deposited two-dimensional MoSe2. 5. Direct and tunable band gap of chemical vapour deposited two-dimensional MoSe2 by layer variation and S incorporation. 6. Synthesis of MoS2 by liquid phases exfoliation and its light emission. 7. Summary and future work.

26. YADAV (Gunjan)
Development of Pure and Doped Gallium Nitride Thin Films Grown Using Laser MBE Technique for the Realization of Photonic and Electronic Devices.
Supervisors: Prof. Monika Tomar
Th26856

Abstract

The recent advancements in the field of photonics and electronics have revolutionized our lives by introducing solid state lighting for general illumination, solar energy harvesting to overcome the energy crisis, fiber-optic devices for faster communication, optical sensors for detection of analytes with high sensitivity, high-resolution displays for better visual effects, transistors for faster switching and for high power and high frequency applications etc. Of all the known semiconductors utilized for photonic and electronic applications, Group-III Nitrides have been majorly studied, with prime focus on Gallium Nitride (GaN). Group-III nitride category comprises of the metal compounds like AlN, GaN, InN along with their alloys. Alloying of these nitrides can help in tuning of band gap, which is one of the primary reasons for the fuelling interest in the utilization of group III nitrides for the development of short wavelength optoelectronic devices like LEDs, photodetectors, solar cells, transistors etc. Currently, device quality nitride thin films are grown by techniques such as MOCVD or MBE, but at considerably high growth temperature (>1000 oC) and in toxic reactive gas atmosphere. Laser molecular beam epitaxy (LMBE) on the other hand is a relatively less explored route for the fabrication of nitride thin films. Thus, in the present thesis, a LMBE technique has been used for the fabrication of Photonic and electronic devices. The present thesis aims towards the development of Photonic (UV Photodetector and LED) and electronic (HEMT, MOS-HEMT, junctionless transistors) devices and their applications in biosensing. For efficient utilization of doped and undoped GaN thin films in photonic and electronic device applications, it is essential to evaluate the variation in values of optical constants with the processing parameters. Photoluminescence spectroscopy and SPR technique are utilized for optical analysis of doped and undoped GaN films. Further, the LMBE technique is used for the growth of fine structured InGaN/GaN quantum well (QW) structures with varying number of quantum well periods for use in various photonic applications such as LEDs,

Solid-state electronics etc. Optical properties were studied using photoluminescence and surface plasmon resonance (SPR) techniques by utilizing the angular examination method in Otto configuration (prism-air gap-metal-dielectric) for samples with a varying number of quantum wells. The optimised thin films of GaN were used to fabricate the high responsivity MSM UV-photodetectors. The effect of different electrodes (transparent and opaque) are used in the fabrication of UV photodetector in lateral configuration. It has been assessed for obtaining high responsivity, high external quantum efficiency, high current ON/OFF ratio and ultra-high detectivity toward UV-A radiations. Further, the InGaN/GaN multi-quantum well (MQW) based conventional and inverted blue ix light-emitting diode (LED) structures are grown using the LMBE technique. Room temperature Photoluminescence (PL) spectroscopy and Electroluminescence (EL) have been performed for the fabricated LEDs. Furthermore, the comparison of high electron mobility transistor (HEMT) and metal oxide semiconductor (MOS)-HEMT were studied. Hafnium oxide (HfO2) is used as a gate dielectric because of its high dielectric constant, high refractive index, high thermal and chemical stability. RF analysis has been performed to analyse the important figure of merits (FOMs) like cut-off frequency, transconductance and gate capacitance of the fabricated devices. An electrolyte gated GaN:Al/GaN HEMT in D-mode and E-mode for electrical detection of uric acid is realized. The proposed EG-HEMT based sensing platform exhibited high sensitivity in a wide uric acid range from 0.1 mM to 1 mM and low detection limit for D-HEMT and E-HEMT were calculated. The stability, reproducibility and interference studies were carried out to know the performance of the device. Further, a planar GaN-based junctionless transistor (JLT) with Hafnium dioxide (HfO2) as the gate dielectric has been fabricated and characterized. Focus of the present work is on a planar and easy to fabricate GaN-on-HfO2 JLT with GaN layer thinned down to 10 nm. The fabricated JLT device was used for fabrication of uric acid biosensor. The device was tested for pH sensing and the maximum pH sensitivity has been chosen for uric acid sensing in the uric acid sensing varying from 0.1 mM to 1.0 mM. Finally, the fabrication of Gallium Nitride based triboelectric nanogenerators (TENG) for energy harvesting from moving NaCl droplets of various concentrations between 0.1 M and 1.0 M is reported. The effect of ultraviolet (UV) light on the DB-TENG has also been studied to enhance the induced signal and the maximum output voltage, current and maximum output power were measured with load resistance.

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