CHAPTER 37

PHYSICS AND ASTROPHYSICS

Doctoral Theses

01. ANJALI RANI

Exploration of Multinucleon Transfer and Fusion Reaction Dynamics in the Vicinity of the Coulomb Barrier for 28Si + 116,120,124Sn systems.

Supervisor: Prof. Samit Kr. Mandal

Th 27692

Abstract

The present thesis encompasses a comprehensive investigation to elucidate the role of multi-neutron transfer channels on the fusion reaction dynamics for 28Si + 116,120,124Sn systems. The fusion and complementary quasi-elastic scattering excitation functions for 28Si + 116,120,124Sn systems were measured spanning ≈15% around the Coulomb barrier using the Heavy Ion Reaction Analyzer (HIRA) at the Inter-University Accelerator Centre (IUAC), New Delhi. The extracted fusion cross sections for the investigated systems at sub-barrier energies were significantly enhanced as compared to the theoretical predictions of 1-D BPM calculations. Various theoretical models based on the coupled-channel (CC) approach (Quantum mechanical and semi-classical) have been employed to probe the underlying mechanism responsible for the observed sub-barrier fusion enhancement. The influence of multi-neutron transfer channels was highlighted in the coupled-channels calculations, particularly for the 28Si + 124Sn system. The extracted fusion and quasi-elastic barrier distribution also reflected the role of multi-neutron transfer channels on the reaction dynamics. The multi-nucleon transfer measurements were performed at and below the Coulomb barrier. The extracted transfer probability in the 28Si + 124Sn system system was comparatively higher than its counterpart's isotopes which signifies the correlation between the sub-barrier fusion enhancement and neutron transfer channel coupling around the Coulomb barrier. The sequential and simultaneous transfer aspect of the extracted probabilities signals the pairing correlation among the participating nuclei. The present thesis also includes the development of a ΔE-E telescope for event-by-event particle tracking and unambiguous identification of mass (A) and charge (Z) of reaction products in a heavy-ion induced reaction. The various design parameters of the detector assembly (a segmented Ionization Chamber (IC) and a Double-sided Silicon detector (DSSD)) viz. geometry, thickness, the distance between electrodes, and operating conditions along with the transport of particles inside the detector have been optimized using GEANT4 and GARFIELD++ interfaces.

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02. ANUJ

Nuclear Structure Studies of Transitional Nuclei in the Mass A~85Region: Yrast and Non-Yrast Phenomena.

Supervisor: Prof. Suresh Kumar

Th 27695

Abstract

In the present thesis, the nuclear structure of ^{84}Sr and ^{85,86}Rb nuclei was investigated by performing three experiments using the Indian National Gamma Array(INGA) at different pelletron facilities in India. Experimental data analysis included γ-ray transition placement in level schemes via coincidence and anti-coincidence relations, relative intensity measurements, and spin-parity assignment using the DCO and polarization asymmetry measurements. In ^{84}Sr nucleus, ten(10) new γ-ray transitions were added, and the γ-band was interpreted as γ-rigid based on the pattern of $S(I)$ behavior. The comparative study of observables suggests an octupole correlation in ^{84}Sr. Large Scale Shell Model(LSSM) calculations were performed for ^{85,86}Rb nuclei using JUN45 and GWBXG interactions. In ^{85}Rb, two(02) new γ-ray transitions were added, and spin-parity was confirmed for previously known levels. Shell model calculations based on both interactions closely predicted negative parity states upto $I^{\pi}=\frac{21}{2}^-$. The JUN45 interaction results for $I^{\pi}>\frac{21}{2}^-$ lie reasonably close to experimental energies, exhibiting similar structure as in $^{87}_{39}$Y$_{48}$ isotone. In ^{86}Rb nucleus, spin and parity were confirmed for all levels above 6^{-} isomer, except at 6798.7 keV level. The $E1$ character for 1427.9-, 1813.3-, and 1880.6 keV, D character for 287.7 keV, and $M1+E2$ character for the 957.2 and 446.9 keV transitions, support $I^{\pi} = 11^+$, 15^+ and 16^+ for 3865.5-, 7412.1-, and 7859.0 keV levels. The $I^{\pi} = 2^-$, 7^- and $I^{\pi} \geq12^-$ states have identical configurations in both interactions. In JUN45 interaction, 10^+_1, 11^+_1, and 12^+ states have dominant contributions that come from a similar configuration, whereas 7^+, 8^+ and 9_1^+ states are produced via the one proton excitation from $2p_{3/2}$ to $1f_{5/2}$ orbitals. For 14^+ and 15^+ states, proton excitation to both $2p_{1/2}$ and $1g_{9/2}$ orbitals, and for 16^+ state, a neutron excitation from $1g_{9/2}$ to $2d_{5/2}$ is required.

Contents

03. ARTI

Investigation of Ferroelectric and Optical Properties of Bismuth Ferrites for Photovoltaic and Photocatalytic Applications.

Supervisor: Prof. Vivek Kumar Verma

Th 27696

Abstract

The present work emphasis on the investigation of the photovoltaic and photocatalytic properties of Bismuth Ferrite (BiFeO3). An overview of the current energy crisis and the necessity to move to renewable energy sources, introduction of photovoltaic solar cells is provided. A thorough evaluation of the photovoltaic and

photocatalytic effects in Bismuth ferrite-based materials has been incorporated. Sample preparation methods are briefly discussed, along with the materials and methods used to characterize the samples after they have been prepared. Single phase Bi1-xPrxFeO3 (x = 0.00 to 0.20) ceramics have been made using the sol-gel. The samples P-E loop analysis demonstrates how Pr doping altered the ferroelectric behaviour. Also, decrease in band gap values of pristine Bismuth ferrite (BiFeO3) with doping has been observed. Energy band gap, Eg = 2.44 eV for BFO energy band gap values reduced to, Eg = 2.27 eV for samples with Pr = 0.15. All these improvement in ferroelectric and optical properties can contribute to photovoltaic applications. Also, photocatalytic efficiency of degrading methylene blue (MB) of Pr doped samples have been noted. Samples of pure and Mn-doped bismuth ferrites [BiFe1-xMnxO3] (x= 0.05,0.10,0.15,0.20) were made using the sol-gel method. In Mn doped samples, ferroelectric and optical characteristics showed a noticeable improvement. The photocurrent density in Mn doped BFO samples was increased. Improved optical properties and ferroelectric of Bi1-xAxFe1-yByO3 samples (A = Pr and B = Mn, Co, Cr) (x = 0, y = 0 and x = 0.15, y = 0.05) by doping with suitable elements has been investigated. Co-doped bismuth ferrite has improved range of polarisation values is from 0.067 to 0.904 μC/cm2. The reduced optical band-gap of BFO, from Eg ~ 2.23 eV to Eg ~1.59 eV has been observed. All this results in better photovoltaic and photocatalytic response in BFO. Bismuth ferrite samples has been co-doped with rare earth (Gd) and transition elements (Mn, Co, and Cr) have been synthesized using the sol-gel method at low temperatures. Doped BFO samples showed an increase in residual polarisation, with the Gd doped BFO sample showing the highest Pr of 1.615 C/cm2. Band-gap values with doping have been found to decrease from Eg = 2.35eV to Eg =1.90eV for Bi0.9Gd0.1FeO3 samples. Enhanced photocurrent response with doping shows better photovoltaic capabilities as compared to pure BFO in doped samples. Co-doping of rare earth and transition elements in bismuth ferrites has been found to increase photocatalytic efficiency levels (η ~ 90.89 % to 96.08%). At last thesis summarizes the results obtained in the present investigations on “Investigation of Ferroelectric and Optical properties of Bismuth Ferrites for Photovoltaic and Photocatalytic applications,” comparative studies and future scope of work on present investigations.

Contents

1. Introduction, literature review and aim of present work 2. Experimental and characterization techniques 3. Improved structural, ferroelectric, magnetic and optical properties of Pr doped multiferroic bismuth ferrites for photovoltaic and photocatalytic applications 4. Improvement in photovoltaic and photocatalytic response of bismuth ferrite by tuning its structural, ferroelectric and bandgap properties 5. Enhanced photovoltaic and sunlight driven photocatalysis for water purification study of rare earth and transition element doped bismuth ferrites 6. Modification in photovoltaic and photocatalytic properties of bismuth ferrites by tailoring band-gap and ferroelectric properties 7. Summary and future aspects. Publications.

04. BHARADWAJ (Hrishabh)
Beyond Standard Model Interactions of Charged Leptons.
Supervisor: Prof. Sukanta Dutta and Sourov Roy
Th 27697

Abstract

par We analyse the beyond Standard Model (SM) interactions of charged leptons to explain the two most challenging phenomena of particle physics. \par My first study

hunts for real spin 0, 1, and 1/2 Dark Matter (DM) candidates primarily interacting with SM-charged leptons through scalar, vector, and twist-2 tensor currents in the domain of effective field theory. Astrophysical observations, LEP data, indirect and direct detection experiments are then used to impose constraints on the Wilson coefficients. \par The discovery potential of DM pairs with mono-photons is studied at the proposed 250, 500, and 1000 GeV c.m. energy International Linear Collider (ILC). The sensitivity analysis of the effective couplings {\it w.r.t.} DM mass reveals that the ILC can be significant in constraining the cosmologically allowed twist-2 and axial-vector Wilson coefficients. \par In the second analysis, we extend the generic leptophilic 2HDM with a singlet complex scalar field and a singlet vector-like lepton. The second scalar doublet does not acquire a VEV in contrast to the SM-like first doublet. We address the theoretical constraints on the model parameters, including vacuum stability, along with the diagonalization of the mass matrix for CP-even, CP-odd, and charged scalars. Constraints on the model parameters arising from precision measurements, LEP, and Higgs decays are discussed. \par We analyse the contribution of the extended inert leptophilic 2HDM to explain the observed disparity in leptons` anomalous magnetic dipole moment (MDM). Using the LHC and LEP constrained aforementioned model, the simultaneous explanation of the MDM of electrons and muons is explored. One-loop diagrams and two-loop Barr-Zee diagrams are taken into consideration in order to carry out this investigation. We observe that the model satisfactorily explains the observed MDM for both electron and muon simultaneously.

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05. CHAKRABORTY (Kajol)
Exploring the Influence of Shell Closure on Fission Dynamics of Nuclei in Mass 200 Region.
Supervisor: Prof. Samit Kr. Mandal and Punita Verma
Th 27699

Abstract

Present thesis investigates the role of dynamic and static shell effects on fission dynamics of nuclei in mass 200 (Hg-Pb-Th) region. Dynamic shell effects influence the early collective motion of dinuclear system before compound nucleus achieves complete equilibrium. Static shell effects become a crucial variable once equilibrium is attained. The first part of the thesis centers on examining the significance of dynamic shell structure effects on fission dynamics via pre-scission neutron multiplicity (νpre) measurements. The νpre values of 220,222,224Th nuclei populated with shell closed entrance channel partners (16O + 204,206,208Pb) reveal considerable impact of entrance channel magicity on pre-fission neutron emission. Systematic statistical model analysis of νpre data including the dynamical effects of collision partners for 28 fusion-fission reactions highlights a hindered pathway to fission for systems with shell closed nuclei in the entrance channel. The second part of the thesis targets towards investigation of the impact of static shell effects in fission of 201,203,205Bi nuclei populated via 19F + 182,184,186W reactions. Unanticipated signatures of asymmetric fission are observed for 203,205Bi upto high excitation energy (E∗) of ≈ 113 MeV. Two-dimensional Langevin model calculations reproduce a fission trajectory that replicates the experimental mass-asymmetry, revealing the role of deformed proton shell closures (Z = 34−38). Prevalent E∗

dependent pre-saddle neutron emission is analysed in terms of increased hindrance in fission pathway due to shell closure. The investigations highlight distinct fission pathways for pre-actindes and actinides, particularly from saddle to scission. The third part of the thesis includes simulation of a ΔE-E telescope, consisting of Multi Wire Proportional Counter, segmented Ionization Chamber and n-type Silicon detector. An energy resolution of 100 keV for a 5 MeV α particle with flight path of 30 cm is optimized. Additionally, the design of a high vacuum chamber required for testing various components of telescope is also optimized.

Contents

1. Introduction 2. Theoretical Formalism 3. Pre-Scission Neutron Multiplicity Systematics: Role of Entrance Channel Shell Closure 4. Experimental Details and Methodology 5. Mass Distribution Measurements of 203,205Bi 6. Neutron Multiplicity Measurements of 201,203,205Bi 7. Instrumentation 8. Summary and Future Outlook.

06. CHANCHAL
Studies on In2Se3 Thin Films and 2D Layered Structures for Device Applications.
Supervisor: Prof. Pradip Kumar Jha
Th 27700

Abstract

In the modern age, the miniaturization offers greater density and shorter signal paths enabling higher frequencies and fast response of the devices. This makes 2D materials, an attractive field of research for next generation device application. Indium selenide (In2Se3) is known to exist in three room temperature stable phases (α, β, γ). α-In2Se3 and β-In2Se3 are the layered phases with bandgap varying from bulk to monolayer in the range of 1.45 - 2.80 eV and 1.3 - 1.55 eV, respectively. α-In2Se3 is also a room temperature ferroelectric 2D materials. γ-In2Se3 is a non-layered semiconductor having a direct bandgap of 1.93 eV. In2Se3 has a high absorption coefficient, carrier mobility and electrical conductivity with a low thermal conductivity, high chemical stability and ferroelectricity, which makes it suitable for the optoelectronic, thermoelectric, sensing and memory device applications. The structural and electronic properties were analysed using density functional theory (DFT). The device performance of In2Se3 is observed to get affected by the defects. Therefore, on the basis of the formation energies under In-rich and Se-rich thermodynamic growth conditions for the intrinsic point defects in all three phases of In2Se3 are analysed. Thin films of In2Se3 are grown using pulsed laser deposition technique and observed that the deposition pressure plays a crucial role in the phase-defined growth of In2Se3. A high performance self-powered UV photodetector is prepared using the as grown In2Se3 thin films owing to its ferroelectricity. The influence of post deposition annealing was studied on the thermoelectric effect-based waste heat conversion and compared with theoretical values calculated by solving Boltzmann transport equation. Then, photoelectrochemical based solar-to-hydrogen conversion and a mediator-less Uric acid biosensing is performed. Next, the number of layers of α-In2Se3 are optimized using PLD and utilized for the self-rectifying and self-selector charge-trap based resistive switching device application.

Contents

1. Introduction to 2D materials and material of choice: In2Se3 2. Study of structural and electronic properties & intrinsic point defects in In2Se3 using DFT

3. Growth and characterization of In2Se3 thin films and 2D layered structures 4. In2Se3 thin films for UV photodetection application 5. In2Se3 thin films for thermoelectric devices 6. In2Se3 thin films for photoelectrochemical cell based solar-to-hydrogen conversion and uric acid biosensing device application 7. Resistive switching in In2Se3 thin films for memory device application. Scope and Suggestions.

07. DEV (Kapil)

Investigation of Magnetization Reversal and Dynamics of Fe-Ni Based Alloys using MOKE and FMR for Spintronics Applications.

Supervisor: Prof. S. Annapoorni

Th 27702

Abstract

Modern data driven world demands more efficient data storage and processing technologies as the traditional devices face limitations of storage density and slow operational speeds. Spintronics based devices, that utilize the electron`s spin along with charge, hold the promise to overcome these challenges and can provide faster processing and enhanced storage capacity at reduced power. This thesis investigates magnetic and magneto dynamic properties of Fe-Ni-based alloys, focusing their potential for spintronics devices. The research begins with the polyol synthesis of spherical permalloy (Fe21Ni79) NPs, and investigating their magnetic and thermal stability in ambient conditions. These NPs exhibit enhanced soft magnetic properties and structural integrity upon annealing. Also, they retained their magnetic properties for a longer duration and proved their chemical and thermal stability up to 350 ˚C in ambient conditions, suitable for magnetic hyperthermia cancer treatment. The thesis further investigates the magnetization switching and dynamics of electrodeposited Fe-Ni alloy thin films. The electrodeposition parameters were adjusted to get high quality, composition-controlled alloy films. The Fe:Ni alloy composition of the films influences the surface anisotropy, domains, magnetization switching and magneto-dynamic behaviour. For electrodeposited permalloy thin films, lowest coercivity, minimum switching field and Gilbert damping was achieved. After heat treatment, the coercivity and switching field reduced to 5 Oe and Gilbert damping reduced to 0.018. Further, the analysis of Fe-Co and Fe-Co-Ni alloy thin films underscores the impact of Ni concentration on domain structures and magnetization reversal processes, offering insights into material optimization for spintronics. Finally, the role of permalloy layer thickness in exchange-coupled Fe-Ni/FePt bilayers, demonstrates how variations in thickness can fine-tune the coercivity for ultrahigh-density storage applications. These findings contribute to the advancement of spintronic technology, paving the way for the development of next-generation memory and processing devices with improved efficiency and performance.

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08. DIMRI (Mayank)
Study of Atomic Processes for Multi-Charged Ions for Plasma Diagnostics.
Supervisors: Prof. Avindra Kumar Singh and Sultana N. Nahar
Th 27701

Abstract

Atomic Physics plays a key role in understanding all branches of Physics. Spectroscopy is an important tool for the development of atomic physics. The field of atomic data covers a wide range of topics from the atomic structure and spectroscopy of atoms/ions to the cross sections which control the rates of processes when these species collide and react in a hot gas/plasma. A great wealth of information regarding the temperature, density and composition of the remote sources can be gained from the detailed analysis of the light emitted by these sources. The demand for atomic data is usually met by direct laboratory measurements of transition wavelengths, intensities and cross sections. However, such measurements are sometimes either not feasible or become very expensive. In that case, theoretical calculations play an important role. For several decades, significant efforts have been made by theoretical atomic physicists for the development of different approaches such as configuration interaction method (CIV3), multiconfiguration Dirac-Fock (MCDF) technique and R-matrix method for calculating large amount of reliable atomic data. In the present thesis, we have presented atomic structure and electron impact excitation scattering calculations for highly charged ions. We have calculated level energies, oscillator strengths and transition probabilities for Na-like Cr XIV ion using the configuration interaction (CI) method CIV3. We have also presented excitation energies, radiative decay rates, oscillator strengths, line strengths and lifetimes for S-like Kr XXI ion using the MCDF method. Further, the plasma screening effects on the atomic structure of He- and Be-like ions embedded in strongly coupled plasma have also been studied. Moreover, we have employed the state-of-the-art R-matrix technique for studying the electron impact excitation of Na-like Cu XIX. The results of the present study should be of great help in the modeling and interpretation of spectral properties in laboratory and astrophysical plasmas.

Contents

09. GUPTA (Gaurav)
Investigations of The Microstructure and Defects in The Wide Bandgap Semiconductors, 4h-Sic and Znmgo.
Supervisor: Prof. Shyama Rath
Th 27703

Abstract

The thesis focuses on the microstructural investigations of two wide bandgap semiconductors, namely silicon carbide (SiC) and zinc magnesium oxide (ZnMgO) along with some of their multifunctional properties. SiC is emerging as a viable alternative to diamond as a host for defect qubits relevant for quantum technologies. The impingement of energetic ions provides one protocol for generating a variety of point defects such as vacancies, divacancies, vacancy clusters, and vacancy-

impurity complexes. In this work, the 4H-polytype of SiC is implanted with 200 keV Si ions at various fluences to generate such defects. The ion implantation induced disorder and the recovery after thermal annealing are assessed through high-resolution x-ray diffraction, Rutherford backscattering spectroscopy and Raman spectroscopy. Photoluminescence spectroscopy is used to investigate some of the optically addressable defects (color centres). Preliminary density functional theory calculations have been undertaken to investigate the defect formation energy. ZnO has been widely investigated for UV optoelectronics. Mg incorporation to form ZnMgO alloy can further extend the optical bandgap deeper into the UV region. However, the structural difference and the large lattice mismatch between ZnO and MgO limit the solubility. In this work, different synthesis methods like ball-milling, green synthesis, and sol-gel auto combustion are explored to increase the solubility of Mg and, consequently, modulate the bandgap in ZnMgO. The microstructural modifications due to Mg incorporation are investigated using Rietveld refinement of x-ray diffraction and Raman spectroscopy. The bandgap and defects are probed through UV-VIS and photoluminescence spectroscopy. Both ball-milled and green synthesized samples give a maximum solubility limit of 10% of Mg. The sol-gel auto combustion method results in a solubility enhancement of up to 20 % of Mg and significantly increases the optical bandgap by 460 meV. The multifunctional properties such as electrochemical, magnetic, antioxidant and antibacterial activity are also investigated.

Contents

10. GUPTA (VISHAL)
Investigation of Organic Polymers for Solar cells and Flexible sensors.
Supervisor: Dr. Lalit Kumar
Th 27704

Abstract

This thesis primarily focuses on the applications of organic polymers in the field of solar cells and flexible sensors. Chapter 1 provides a foundational introduction to organic polymers, describing their distinctive properties and versatile applications. This chapter extends to offer a comprehensive overview of organic solar cells (OSCs), ultraviolet (UV)-blocking sheets, gas sensors and electrochemical detectors, providing insightful explanations of their underlying operational principles. Chapter 2 offers an in-depth exploration of the principles governing characterization and measurement techniques applied to study the diverse properties of materials. Additionally, the chapter thoroughly examines various deposition techniques utilized for material deposition, providing a comprehensive understanding of the methodologies employed in the research. Chapter 3 reports the development of an indium tin oxide (ITO)-free plasmonic-assisted inverted OSC. The aluminium-doped zinc oxide (AZO) front cathode prevents the degradation of organic solar cells from harmful UV rays and the introduction of plasmonic gold nanoflowers within the active layer enhances the power conversion efficiency of the device. Chapter 4

investigates free-standing flexible sheets of zinc oxide/poly(methyl methacrylate) (ZnO/PMMA) nanocomposite for their UV-blocking characteristics. ZnO nanoparticles of varying sizes (25 to 200 nm) are prepared with the sol-gel method, and their dispersion in PMMA is used to obtain transparent ZnO/PMMA free-standing flexible sheets. Chapter 5 introduces an efficient, flexible, and affordable ammonia (NH3) gas sensor fabricated over a biodegradable paper substrate. The active sensing material, polyaniline (PANI) film, is deposited via a simple in-situ polymerization technique and its optimization is done to detect NH3 gas. Chapter 6 presents a novel label-free electrochemical sensor to detect bisphenol A (BPA) using PANI film deposited on a flexible polyethylene terephthalate (PET) substrate. The sensor demonstrates linear characteristics in the concentration range of 0.05 - 5.0 μM, with high sensitivity and a low limit of detection. The sensor exhibits flexibility, long shelf life, and proves to be a promising candidate for an electrochemical-based BPA sensor. Chapter 7 provides a concise overview of the potential future research directions for this work.

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11. JITENDRA KUMAR
Exploring Neuronal Membrane Complexity Mathematical Models for Nonlinear Capacitance of Axonal Membrane and Cooperative Ion Channel Interactions.
Supervisors: Prof. Awadhesh Prasad, Patrick Dasgupta and Subhendu Ghosh
Th 27705

Abstract

The axonal membrane of a neuron plays an important role in the generation and propagation of action potential. The axonal membrane can be represented as the electronic capacitor and embedded proteins (ion channels) as the resistance. The reported mathematical models for neurons, e.g. Hodgkin-Huxley (HH) model, presented the membrane capacitance as a constant parameter. However, the membrane capacitance has been shown to have a nonlinear dependence on the cell membrane potential in various types of cells. In the present work, the axonal membrane capacitance has been considered as nonlinear and its effect has been studied in three different types of neurons, e.g. squid giant neuron, rodent hippocampal interneuron, and rodent cortical neuron using the Hodgkin-Huxley model. The simulated results indicate a reduction in the firing rate of the neurons after a critical value of the nonlinear capacitance. Simultaneously the inter-spike interval (ISI) changes with the nonlinear membrane capacitance. Similarly, voltage-gated ion channels play an important role in generating action potential in neurons. These ion channels are found to be in localized cluster form on the axonal membrane surface and behave cooperatively. However, in Hodgkin-Huxley`s model of action potential, the ion channels are considered to function independently. According to some recent reports, the activity of an ion channel is influenced by the neighbouring ion channel activities. Herein, the HH model has been modified based on our previous studies on cooperativity among ion channels. Computational analysis of the proposed model shows that the initiation of the action potential, amplitude, and hyperpolarization is affected significantly by the cooperative

interactions among the voltage-gated ion channels present on the axonal membrane surface. Finally, the combined impact of nonlinear membrane capacitance and cooperativity in ion channels was studied which led to results similar to single-factor scenarios (the above-mentioned studies), but with some quantitative differences. These results are qualitatively supported by the existing experimental facts.

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12. KAKKAR (Astha)
Partition Functions and Phases of Quantum Field Theories in Anti-de Sitter Spaces.
Supervisors: Prof. Supriya K. Kar and Prof. Swarnendu Sarkar
Th 27706

Abstract

In this thesis we present a new method to construct one-loop partition functions for scalars, fermions and U(1) vectors in (d+1) dimensional AdS spaces for arbitrary d. Our method utilizes eigenfunctions of Laplacian, Dirac and vector Laplacian operators on Euclidean AdS in Poincare coordinates and method of images. For finite temperature, partition functions are obtained by generalizing eigenfunctions to obey desired periodicities (anti-periodicities) for bosons (fermions) under quotient group action defining thermal AdS. The results obtained match with those available in literature obtained using other methods. We then study phases of scalar field theories in thermal AdS spaces for d=1,2,3. The analysis is done for theories with global O(N) symmetry for finite and large N. Symmetry preserving/breaking phases are identified as function of mass-squared of scalar field and temperature. We highlight deviations from corresponding flat space results. We next study phases of Yukawa theories at one-loop for d=1,2,3 and Gross-Neveu models for d=1,2 in AdS spaces at zero and finite temperature. We study phases of these fermionic theories as regions in corresponding parameter spaces at zero temperature. Phases and phase boundaries are further identified as function of mass-squared of scalar field and temperature for Yukawa theories. For Gross-Neveu models, changes in phases as function of fermionic mass and coupling constant at finite temperature are discussed. Gross-Neveu-Yukawa model is studied for d=4. We note certain deviations from phases in flat space. For U(1) vectors, we analyze phases of scalar QED theories at one-loop in d=2,3 first for single scalar QED theory as functions of AdS radius at zero temperature showing that results reduce to those in flat space in large AdS radius limit. Thereafter phases are studied as function of scalar mass and temperature. We also derive effective potentials and study phases of scalar QED theory with N scalars.

13. MOHIT
Investigations on Sodium Ion Capacitors Fabricated with Dual Carbon Electrodes and Porous Polymer Electrolytes.
Supervisor: Prof. S.A.Hashmi
Th 27704

Abstract

The demand for energy to meet the needs of the global community has increased many-fold as the world population has grown and the global economy has developed. To harness the full potential of energy sources, we need efficient energy storage devices. Lithium-ion batteries (LIBs) are most prominently used for energy storage. However, the most important component of LIBs, lithium has a non-uniform distribution in the earth`s crust (0.065%), and it is mostly found in politically unstable regions with severe geographic conditions. The sodium-ion battery (NIB) offers an alternate solution to this lithium problem because of its large availability and low cost. Electrical double layer capacitors (EDLCs) are widely investigated class of supercapacitors, which have ability to deliver high power, however, their specific energy is generally low (<5 Wh kg-1). The present thesis presents the detailed preparation and characterization of two types of activated carbon electrode materials and hard carbon anode from pre-treated biomass sugarcane bagasse, preparation and characterization of environment friendly porous polymer electrolyte, and characterization of an eco-friendly Na-ion capacitor (NIC). The Na-ion capacitor has been assembled with the optimized anode (Hard carbons), cathode (ACs) and porous electrolyte described above.

Contents

14. NAVEEN
Magnetotransport in Weyl Semimetals: Effect of Disorder and Shape of Fermi Surface on Edge States.
Supervisor: Prof. Navedita Deo
Th 27708

Abstract

The development of Weyl semimetals (WSMs) as a new type of quantum material for a variety of novel phenomena is underway. In this thesis, we have investigated the transport features of thin film WSM with broken time reversal symmetry in the the presence of perpendicular and tilted magnetic field. The equi-energy contours possess a topological invariant called turning number ν. In the first context, Magnetotransport in WSMs, with and without disorder, having turning number of Fermi surface $\nu=0$ and $\nu=1$ are examined. The various shape of Fermi surface are due to two different considerations of model Hamiltonian one with broken inversion symmetry and other with preserved inversion symmetry. This results in exotic Weyl orbits which are a hybrid of bulk and surface states and are crucial for magnetotransport. We numerically investigate the magnetotransport in z-direction when magnetic field is in the x-direction perpendicular to the Weyl semimetal slab. For the first case with broken inversion symmetry we get two counterpropagating states on each edge i.e. one edge has only n-type states and other has only p-type states. When an electron (hole) reservoir is connected to the slab in z-direction, only n-type (p-type) edge channel passes through the contact for an applied bias. For the second case in which inversion symmetry is preserved we get only p-type states on each edge, propagating in the opposite direction at each edge, very similar to 2D quantum Hall effect. The transverse

magnetoconductance is an integer multiple of e^2/h for both the cases. The edges states are not very robust in the presence of disorder for the first case but for the second case, edge states can persist upto a certain value of disorder strength. In the second context, We extend the numerical investigation of the the magnetotransport in the WSM to include systems with the turning number of Fermi surface greater than unity, $\nu = 2$, which is due to the self intersection of equi-energy contours. This is in contrast to the conventional electron gas in which orbits are closed curves without self intersection. In the presence of a perpendicular magnetic field on a slab geometry, the probability density of edge states are wide and narrow on each edge rather than symmetric on both edges. We explore the effect of disorder on the edge states and find that the conductance remains quantized at $2e^2/h$ upto a critical disorder strength. Our findings show that the transport characteristics of WSM are more robust to disorder in a particular direction for these systems with higher turning number. These systems also show unusual conductance by a slanted magnetic field as the slant can modify the Landau levels at the Fermi level. The transverse magnetoconductance in y-direction is found to be robust against the disordered impurity potential which may be the signature of quantum Hall effect in 3D.

Contents

15. NITESH KUMAR

Automated Analysis of Stellar Photometric and Spectroscopic Astronomical Data.

Supervisors: Prof. H. P. Singh & Prof. Philippe Prugniel

Th 27709

Abstract

We present the analysis of stellar photometric and spectroscopic data using machine learning methods. We used artificial neural network (ANN) based interpolation to generate the light curves of RRab stars in the I and V bands based on a pre-computed grid of models. The trained interpolators were used to predict the light curves of RRab stars in Magellanic clouds, and good agreement was found between the observed and predicted light curves. ANN interpolators provide a fast and efficient technique to generate a smooth grid of model light curves for a wide range of physical parameters. We did a comprehensive photometric study of RR Lyrae stars in the M3 globular cluster utilizing a vast dataset of 3140 optical CCD images spanning 35 years from astronomical data archives. The periods of 238 RR Lyrae stars (178 RRab, 49 RRc, and 11 RRd) were improved using the Multiband periodograms. The distance to the M3 globular cluster was derived using period-wesenheit relations calibrated using theoretically predicted relations from literature. The physical parameters of 79 non-Blazhko RRab stars were determined using the ANN based comparison of theoretical and observed light curves. We also applied the ANN to derive the atmospheric parameters of stars in NGC 6397 from their spectra observed from the MUSE spectrograph mounted on a Very Large Telescope (VLT). We trained the ANN to interpolate within the parameter space of the Gottingen Spectral Library (GSL). The trained ANN, used with the spectroscopic analysis software ULySS, provided the atmospheric parameters of observed stars in NGC 6397. The derived atmospheric parameters are in excellent agreement with those provided in the literature.

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16. RAO (Ankit Kumar)
Study of Structurally Modified New Phosphorescent Emitters for Design and Development of Organic Light-Emitting Diodes.
Supervisor: Prof. Amarjeet Kaur
Th 27712

Abstract

Organic light-emitting diode technology, harnessing the potential of phosphorescent materials, offers a promising pathway for developing energy-efficient devices for diverse lighting and display applications. This study delves into the potential of transition metal complexes, particularly iridium-based phosphors through design and development of novel metal complexes utilizing 2-phenylimidazo[1,2-a]pyridine (pip) ligands, known for their thermal and photostability, short excited-state lifetimes, high luminescent quantum yields, and precise color-tuning capabilities. Stuctural conformation of the complexes is conferred through NMR, elemental and FTIR analysis indicating high purity and yield. Further, the study presents a detailed analysis of the particle morphology through SEM analysis, revealing spherical particles (0.13 μm) in $[Ir(ppy)_2(acac)]$ to cubical particles (0.17 μm) in $[Ir(pip)_2(acac)]$, rod-like particles (0.82 μm) in $[Ir(pip)_2(tmd)]$, and granular particles in $[Ir(pip)_2(bza)]$. Thermogravimetric analysis demonstrated that all complexes exhibit thermal stability up to 573 K, with a two-stage decomposition process. The electrical properties of the complexes revealed semiconducting behavior with a transition to metallic behavior at elevated temperatures, driven by the removal of coordinated water molecules. The room temperature conductivity of the samples is approximately ~10-8 S/cm. Theoretical simulations using DFT predict that the novel iridium complexes exhibit a distorted octahedral geometry. The simulated absorption spectra aligns well with the experimental one, exhibiting signature bands in the UV and visible region attributed to π-π* and MLCT transitions. Photoluminesence studies reveal that modifications in the ligands lead to significant shifts in emission spectra i.e. from green to red in the present work, highlighting the influence of structural modifications in ligands on photophysical properties. Electrochemical analyses provide additional depth, illustrating how variations in the ligands influence the HOMO-LUMO levels, thereby affecting the bandgap and emission spectra. Finally, the study showcases the fabrication of OLED devices with varying architectures, achieving significant efficiencies and low turn-on voltages. The lowest observed turn-on voltage of 3V for devices with pip ligands, alongside a maximum efficiency of 13.9%, highlights the effectiveness of the ligand optimization and device architecture.

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Emitting Iridium Metal Complex Based on Benzoyl Acetone Ancillary Ligand 8. Summary and Future Prospects. Annexures.

17. RAVINA
Temperature Dependent Dielectric Response and Luminescence Thermometry in Lanthanum Titanate Ceramics.
Supervisor: Prof. P. Senthil Kumar
Th 27711

Abstract

The present thesis is focused on the (i) preparation and characterisation of La2Ti2O7 ceramics, (ii) analysing the temperature dependent dielectric response, (iii) investigate Bi dopant as a sintering aid, (iv) examine luminescence effects with Er/Yb dopants and (v) explore non-contact sensing of temperature based on upconversion luminescence effect. Sintering at 1600°C produces a dense microstructure and a stable dielectric response ϵ^` (f) with low dielectric loss (~10–3), and low dc conductivity (~ 10−15 Ω–1cm–1). Variations in the electrical properties are correlated with the observed changes in ceramic microstructure. Grain and grain-boundary effects are distinguished by impedance spectroscopy. Usefulness of Bi as a liquid phase sintering agent is clarified with significant reduction of sintering temperatures (1300 °C) and improvements in densification. Site selectivity of Bi and its substitution in La2Ti2O7 is identified by Raman spectroscopy, and improvements in the dielectric and ferroelectric properties are seen for an optimized Bi content. Temperature dependent dielectric response is analysed in the temperature range 123–473 K over a wide frequency range (0.1Hz – 1MHz). Grain, grain-boundary and electrode- polarisation effects are identified from impedance Cole-Cole plots. A broad concavity in DC conductivity versus temperature characteristics in the temperature range 123–153 K reveals the possible interaction between hole-polarons and electrons. Activation energies of EA = 0.33 ± 0.03 eV and EA = 0.54 ± 0.02 eV in the temperature range 153-473K indicate hopping conduction of singly ionised oxygen vacancies. Upconversion luminescence in La2-x-yErxYbyTi2O7 powders and ceramics is analysed. Temperature sensing in the range (93–773K) using luminescence intensity ratio (LIR) method for an optimized Er/Yb dopant concentration (x = 0.025, y = 0.05) has been studied. Sensitivity, responsivity, repeatability and uncertainty for temperature measurement are clarified in the proposed non-contact temperature sensing method using upconversion luminescence

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18. SAINI (Rimpy)
Thin Films of Bismuth and Bismuth Stearate: Synthesis, Structure and Optical Properties.
Supervisor: Dr. Sumalay Roy
Th 27713

Abstract

In the past, many inorganic processes for the synthesis of single and bi-layers of bismuth were reported using physical and chemical vapor deposition techniques.

The ultrathin films deposited are found to interact electronically with the substrates due to their proximity to the substrate surface. We introduce a new and easy organic channel for the synthesis of the bismuth multi-bilayers in ambient conditions. Bismuth stearate multi-bilayer thin films are deposited on the hydrophobic silicon and hydrophilic glass substrates using the Langmuir-Blodgett technique. Optical absorption spectroscopy measurements in the infrared region provided information on various bond structures present in those bismuth stearate thin films. Specular x-ray reflectivity (XRR) experiments and their analysis of such thin films unambiguously show the highly periodic stacking of bismuth bilayers along the surface-normal directions within the multilayer film structure. The morphology of the surface obtained from field emission scanning electron microscopy supports the XRR analysis. A band-gap of 3.2 eV was obtained for such bismuth stearate thin films from the UV-Visible spectroscopy. Apart from the above mentioned organic multi-bilayer of Bismuth, we envisaged another inorganic physical process for deposition of Bismuth thin films. Bismuth thin films of five different nominal thicknesses (below 30 nm) were grown onto silicon (111) by thermal evaporation technique. An extensive and systematic structural investigation of highly oriented Bismuth thin films which carried out. Analysis of x-ray diffraction shows that the crystallite grains of the polycrystalline Bismuth thin films are highly oriented. It is found that the average crystallite size increases, as the film thickness increases. Film thicknesses are accurately determined using the x-ray reflectivity technique. The surface topographies are investigated using atomic force microscopy. Finally, the optical properties of the Bi thin films, which are deposited on glass, are investigated using ultraviolet-visible-near infrared spectroscopy

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19. SHARMA (Prince)
Spectral and Timing Study of X-ray Binaries.
Supervisors: Prof. Anjan Dutta and Chetana Jain
Th 27714

Abstract

This work is based on the detailed spectral and timing analyses of accreting X-ray binaries (XRBs). Accreting XRBs are binary systems comprising of a compact object (neutron star (NS) or black hole (BH)) and an optical star as the companion. The compact object accretes matter converting the gravitational potential energy of the in-falling matter to kinetic energy which eventually gets transformed into electromagnetic radiation, resulting in X-rays. Detailed broadband spectral studies of low-mass X-ray binaries (LMXBs) and high-mass X-ray binaries (HMXBs) have been performed and results have been presented in this thesis. The work focuses on the broadband time-averaged spectral analysis of the NS LMXBs, XTE J1710-281 and 2S 0921-63, utilizing archival data from the Suzaku satellite. The analysis provides a detailed spectral characterization of XTE J1710-281 and 2S 0921-63 up to 30 and 25 keV, respectively, with improved parameter constraints for the first time. In addition to the NS XRBs, spectral study of the black hole candidate (BHC) 4U 1957+11 is also presented to explore the variation of the spin of the BH, with system parameters like mass, inclination, and distance. A detailed spectral and timing study of HMXB pulsars has also been performed as a part of this work. The presence, discovery and evolution of cyclotron line features have been studied in the

spectra of OAO 1657-415, GRO J1750-27, and 4U 1538-522, respectively. In the time domain, the long-term spin period trends of these pulsars have been explored which show that the spin period exhibits periodic variability on time scales of 1744 d and 271 d, for OAO 1657-415 and 4U 1538-522, respectively. A comprehensive discussion has been provided for the observed properties of all the sources.

Contents

1. Introduction 2. Instrumentation and analysis 3. Comptonized spectra of eclipsing LMXBs 4. Spin period evolution and torque reversal 5. Cyclotron features and magnetic field estimation 6. Exploring correlations between system parameters of black hole candidate 7. Summary and future plan.

20. SINGH (Angad Yuvraj)
Modeling Evolution of Protocells Containing Bistable Autocatalytic Sets.
Supervisor: Prof. Sanjay Jain
Th 27715

Abstract

In the origin of life research, how simple prebiotic chemical organisations became more complex remains an unsolved puzzle. Understanding evolutionary capabilities of compartmentalised systems (or protocells) containing simple autocatalytic sets would be an important step in understanding the puzzle. While earlier work has contributed various pieces relevant to protocell modeling, no one has been able to construct a convincing theoretical model that shows that a population of protocells containing autocatalytic sets can exhibit Darwinian evolution in a fixed environment. In this thesis we present a class of mathematical models wherein one can explicitly see the evolution of protocells through a Darwinian process like natural selection. The role of mutations is played by stochastic fluctuations in the population of molecules within protocells. To the existing body of work on protocell models, our work brings two new ingredients: (i) multistability in autocatalytic sets and (ii) a treatment of protocell size dynamics inspired from recent developments in bacterial physiology. This together with the simplicity of our model has enabled us to study dynamics at multiple scales ranging from the population of molecules within protocells to the population of protocells. We explicitly demonstrate the process of and conditions for natural selection in a population of protocells that are missing in earlier models.

Contents

1. Introduction 2. Dynamics of autocatalytic sets 3. Dynamics of a single protocell 4. Dynamics of a population of protocells 5. Towards a more realistic protocell model 6. Summary, future directions and some preliminary investigations. Bibliography

21. SUDIPTA
Unravelling the Potential of Multicomponent Mesoporous Bioactive Glass Nanoparticles: An Approach to Improve Ion Therapy.
Supervisor: Prof. Sevi Murugavel
Th 27716

Abstract

The development of advanced implantable materials is crucial for addressing diverse medical needs, ranging from tissue regeneration to tumor treatment and antibacterial properties. Mesoporous bioactive glasses (MBGs), particularly copper-doped variants (Cu-MBGs), have emerged as key contributors in crafting innovative biomaterials for treating bone defects. Notably, Cu-MBGs excel in promoting bone formation, encouraging blood vessel growth, and displaying, antibacterial effects, making them highly promising for a variety of biomedical applications. The primary objective of the study is to enhance the surface area and Si-OH group density in 82S, 70S and 58S MBG samples through the P123 template removal step, with a particular focus on their biological activities. The ethanol extraction method is employed for sample stabilization. Additionally, the impact of acid and ethanol extraction methods on the textural features of CuO contained 58S MBG is investigated, revealing the superior efficacy of the acid extraction process. The role of catalysts in the sol-gel route is explored with distinct textural, structural and morphological properties observed in different Cu-MBG samples. Comprehensive assessments on bioactivity, hemolysis, antibacterial activity, anticancer activity and biocompatibility are conducted to understand the impact of textural properties and Si-OH density. Various analytical techniques are utilized to analyze the structural, textural and morphological properties of MBG samples before and after in-vitro bioactive test. Overall the findings contribute valuable insights into optimizing the synthesis of MBGs for enhanced biological functionalities.

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22. TAHIR AHMAD

First-Principles Calculations and Experimental Investigations on Multicomponent Oxide Thin Films for Realization of Optical Devices.

Supervisor: Prof. Pradeep Kumar Jha

Th 27693

Abstract

The field of optoelectronics has experienced significant advancements and there is a growing demand for novel materials with enhanced electrical and optical properties. This thesis work aims to combine the first-principles calculations to understand the fundamental aspects of the materials in the pure and doped form and experimental investigations by growing thin films by using PLD technique for electro-optical modulator. For this study two multicomponent materials have been chosen-BiFeO3 (BFO) and Sr0.6Ba0.4Nb2O6 (SBN60). DFT calculations have been carried out to investigate the structural, electronic and optical properties of Cr doped BFO and Ca doped SBN, the stability of the dopants introduced at various sites have been studied using formation energy calculations. The introduction of Cr along with some rare-earth elements at the Fe-site and Bi-site as codopants in BFO have been studied for the photocatalytic properties. The effect of spin-orbit coupling on the electronic and optical properties of BFO has been reported and the resulting splitting in the bandstructure of BFO has been discussed in the light of Rashba and

Dresselhaus effects. The experimental studies are carried out over the pure and doped BFO and SBN thin films. The grown thin films are characterized for their structural, morphological, compositional, electrical and optical properties using XRD, UV-visible spectroscopy, FESEM-EDX and Raman spectroscopy. The ferroelectric properties are studied using the Radiant P-E loop tracer. The spectra obtained using UV-visible spectroscopy is studied by Swanepoel's method and the optical constants like refractive index, extinction coefficient and dielectric constants are calculated in the visible region. The experimentally obtained parameters are compared with the theoretically obtained values. The thin films of pure and doped BFO and SBN60 are investigated for the electro-optic effect and the effect of the dopants on the electro-optic coefficient have been discussed.

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23. VARSHA
Response of Quantum Heterostructures to External Fields.
Supervisor: Prof. Poonam Silotia and Vinod Prasad
Th 27717

Abstract

In this thesis, we have studied the response of a few quantum heterostructures namely quantum dots, quantum rings, etc. to the external fields. In the modern era, low-dimensional semiconductors have a unique place due to their wide applications in new optoelectronic devices, solar cells, light-emitting diodes, lasers, quantum computing, quantum entanglement, communication, and many more. Quantum dots can be fabricated in different shapes like spherical, cylindrical, ring, elliptical, etc. The optical and electronic properties of these quantum heterostructures can be manipulated with external factors (like impurity, external fields, etc.). In addition, the confining potential and confinement size significantly changes the system`s characteristics. Impurities are added to the system to enhance the properties of the quantum dots. The selection of confinement potential is made to approximate a practical model as closely as feasible. The thesis involves the investigations of the energy levels, transition matrix elements, etc. along with the optical response of these systems to the electric and magnetic fields. The focus of the work is on linear, nonlinear optical absorption coefficients, refractive index changes, second harmonic generation, and third harmonic generation in different shaped quantum dots. It is found that optical response greatly depends on many factors like size, shape, strength of confinement potential, etc. Also, the electromagnetically induced transparency using two laser fields, one serving as a probe and the other as a coupler field is detailed. Finally, the spin dynamics including persistent currents in a 2-dimensional quantum ring are presented. Interesting results are found and explained. The numerical methods to solve the time-independent Schro¨dinger equation used are the finite difference method and finite elements methods, whereas the time-dependent Schro¨dinger equation is solved using either the Floquet method or the 4th-order Runge-Kutta method depending on the nature of the problem undertaken.

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24. YADAV (Jatin)
Study of Dissociation Dynamics of Acetylene Molecules.
Supervisor: Prof. Jyoti Rajput
Th 27718

Abstract

The ion-molecule collision experiments were performed and the dissociation dynamics of the acetylene molecular ions induced by ion impact is studied using the Recoil Ion Momentum Spectroscopy. The present thesis work details an experimental investigation into the three-body dissociation pathways of triply charged acetylene ([C_{2}H_{2}]^{3+}) into fragment sets (H^{+}, C^{+} , CH^{+}) and (H^{+} , H^{+} , C_{2}^{+}). The different modes of breakup are identified and compared. The breakup into (H^{+}, C^{+} , CH^{+}) fragments proceed in three ways: concerted breakup in acetylene configuration, concerted breakup in vinylidene configuration and a sequential breakup via [C_{2}H]^{2+} intermediate molecular ion. The contributions from vinylidene configuration is a clear signature of “Hydrogen migration in the triply charged acetylene” and is an counter-intuitive process. The breakup into (H^{+} , H^{+} , C_{2}^{+}) shows only the concerted mode through the asymmetric and symmetric stretch of the C-H coordinate of the [C_{2}H_{2}]^{3+} molecular ion. By collecting events coming exclusively from the sequential breakup leading to (H^{+}, C^{+} , CH^{+}), we have determined the kinetic energy release for the unimolecular fragmentation of the molecular intermediate, [C_{2}H]^{2+} . Ab initio calculations are performed to generate the potential energy surface of the lowest electronic state of [C_{2}H]^{2+}, as a function of C-C and C-H bond stretches, which show the existence of a metastable state with two possible dissociation pathways. The barrier for dissociation via C–C bond break is found to be lower by ≈2.1 eV as compared to dissociation via a C–H bond break. The calculated KER for the unimolecular dissociation of [C_{2}H]^{2+} along the C–C bond stretch matches well with the experimental value, indicating that the lowest electronic state of [C_{2}H]^{2+} ion is populated in our experiment.

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